H. S. Green

Information Theory and Quantum Physics

In this book, H. S. Green, a former student of Max Born and well known as an author in physics and in philosophy of science, presents an individual and modern approach to theoretical physics and related fundamental problems. Starting from first principles, the links between physics and information science are unveiled step by step: modern information theory and the classical theory of the Turing machine are combined to create a new interpretation of quantum computability, which is then applied to field theory, gravitation and submicroscopic measurement theory and culminates in a detailed examination of the role of the conscious observer in physical measurements. The result is a highly readable book that unifies a wide range of scientific knowledge and is essential reading for all scientists and philosophers of science interested in the interpretation and the implications of the interaction between information science and basic physical theories.

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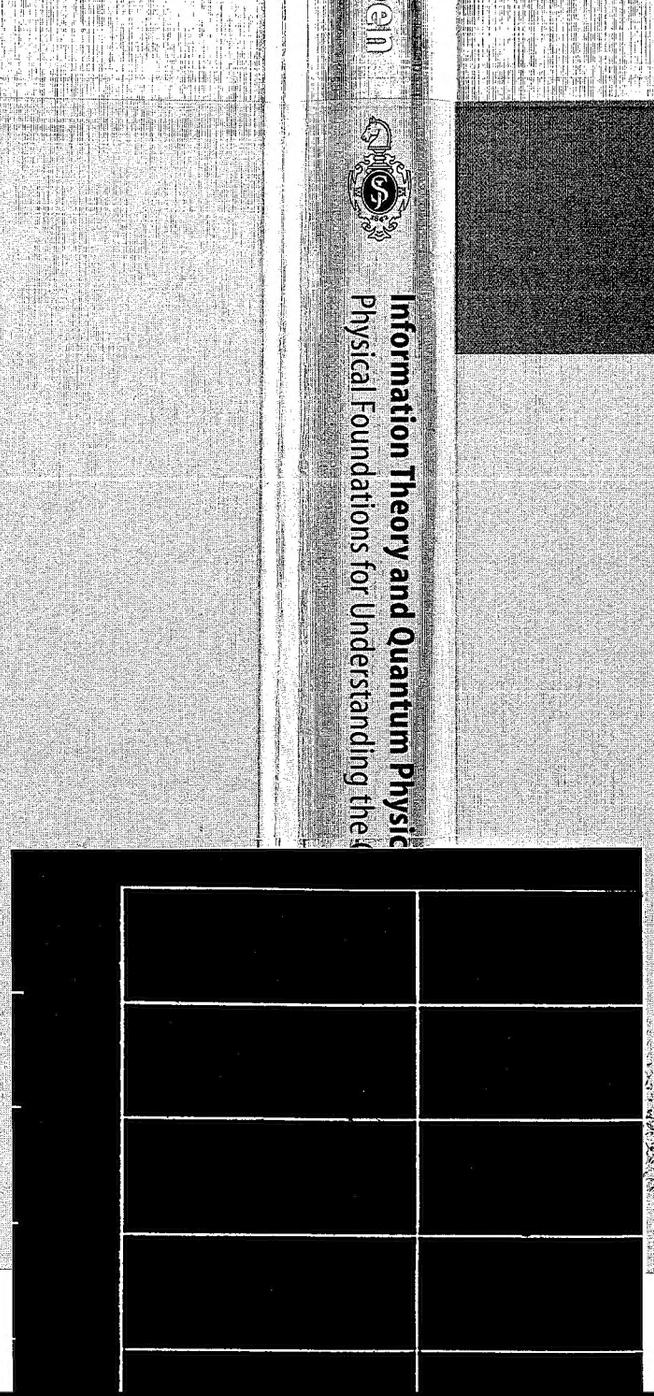

H. S. Green

Information Theory and Quantum Physics

Physical Foundations for Understanding the Conscious Process

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Physical Foundations for Understanding the Conscious Process

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Preface

The approach of a new century is an appropriate time not only to survey the achievements of the past but to study the changes that have taken place in the understanding of these achievements and the way they are likely to affect the future. In physics the twentieth century has been a time of prodigious achievement, resulting at first from the work of a relatively small number of men and women of great distinction raised in the European tradition, but eventually, with the steady growth of a scientifically educated population in many different cultures, attributable to the interaction and cooperation of talented physicists of every description. The most obvious change has been in the volume of literature available, which has by now become so large that no single person can assimilate it. The increase in volume is to some extent associated with the penetration of physics, by now largely quantum physics, into other sciences so as to embrace quantum chemistry, quantum biology, and quantum computation. The understanding of physics is also in the process of rapid change, brought about largely by the unprecedented development of digital computing and by the concurrent dissemination of information.

On the other hand, the close relation between physics and information theory, which was evolved only rather late in the century, is still not widely appreciated, and one of the aims of this book is to demonstrate the fundamental simplicity of an approach which brings together the two disciplines. But perhaps even more important is an appreciation of the role of the conscious human observer of the universe of shared perception. Unless this role is taken into account, information theory is easily seen to be no more than an application of the mathematical theory of probabilty. The laws of quantum mechanics are widely accepted as intimately related to the phenomenon of consciousness, and will be shown to be so in the penultimate chapter of this book, where effective definitions and a physically based theory will finally emerge. But quantum physics implies quantal information, and it is to be hoped that an essentially simple account of their mutual relations may help to facilitate an understanding of each of these rapidly developing areas and help to disentangle ideas based on significant information, available to any observer, from those which are simply a matter of personal preference.

The exclusion from the text of formal exercises and references to the literature is a deliberate departure from custom. In compensation, the reader is

invited to investigate the truth of a variety of statements scattered through the text which are preceded by an asterisk, and is recommended to seek additonal information on any topic from a highly selective list of publications to be found at the end of the text and in the Appendix.

South Australia, Australia 1998 *H.S. Green*

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1. First Principles

In the past, science has often been presented as a system of natural laws that are the product of experience and may be used as a rational basis for prediction. The laws were the laws of geometry, as formulated by the ancient Greeks, the laws of motion and gravitation, as formulated by Newton, and the laws of electricity and magnetism, as formulated by Faraday and Maxwell. During the twentieth century, however, these laws were found to be inexact and therefore unreliable in certain circumstances. Einstein's theory of relativity first suggested the need for the revision of the laws of Euclidean geometry, Newtonian mechanics and gravitation; the discovery of quantum mechanics led to further changes, and classical and quantized field theories were developed in which the laws of electromagnetism were subordinate to more general gauge theories.

It can never be certain that the laws of physics have reached their final form, and it is therefore of considerable importance to isolate those general principles underlying mathematical and theoretical physics which have been and seem likely to remain unaffected by change. To some extent these principles are the refinement of experience, in the sense that they are derived from experiment and observation, but inevitably they have also been influenced by the imagination of the conscious mind. The interplay of observation and imagination is a vital prerequisite of science. But to avoid the intrusion of purely imaginary concepts a philosophical principle known as 'Occam's razor' is of fundamental importance. In the language of William of Occam, this was: "It is vain to do with more what can be done with less", and carried the implication that if the observed facts can be accounted for without a certain hypothesis, that hypothesis should not be accepted! The principles of physics which appear to survive this test are the subject of the separate sections of this chapter.

1.1 Relativity and Equivalence

The **Principle of Relativity**, the fundamental importance of which was first recognized by Einstein near the beginning of the twentieth century, may be stated as follows: *The laws of physics are the same for every force-free observer.* Initially these laws included only Newton's laws of motion and

the laws of electricity and magnetism, but no essential difficulty was found subsequently in reconciling all the laws of particle physics with the Principle.

A significant feature of the Principle of Relativity was its recognition of the role of the observer. However, in practice no distinction was made between the observer and the means of observation, which was idealized as what is known as an *inertial system.* The distinction between the observer and the associated observational system is in fact important only when the phenomenon of consciousness, which for a long time was hardly understood, is taken into account, and we shall therefore consider an inertial system to be associated with a particular observer at a particular time. There is an inertial system, which we shall denote by (0), corresponding to an observer considered to be at rest at a fixed point of space, called the *origin.* Another inertial system (x) is completely specified by the position $\mathbf{x}$ of its centre of mass at time t, its orientation $\mathbf{u}$ and its velocity $\mathbf{v}$ relative to the inertial system (0). If the cartesian components of the vectors $\mathbf{x}$, $\mathbf{u}$ and $\mathbf{v}$ are denoted by (x^1, x^2, x^3), (x^4, x^5, x^6) and (x^7, x^8, x^9) respectively and the time t by x^0, the 10 parameters x^d $(d = 0, 1, 2, ...9)$ specify the relation between the inertial systems (x) and (0). The parameters are, in principle, macroscopic quantities measured in the inertial system (0). The magnitude u of the vector $\mathbf{u}$ is the angle through which the inertial system (0) must be rotated, about an axis along $\mathbf{u}$, to give it the same orientation as (x). The x^d for $d = 0, 1, 2, ...6$ are therefore all *geometrical* parameters, whereas for $d = 7, 8, 9$ they are *kinematical.* They all depend on the choice of origin, and therefore subject to *geometrical and kinematical transformations* if the origin is changed.

The gravitational, electromagnetic and other potentials from which forces are calculated also have arbitrary components, called *gauge potentials*, the choice of which in a particular inertial frame is said to fix the *gauge.* The values of the gauge potentials $(\varphi^1, \varphi^2, ...)$ at the point $\mathbf{x}$ and the time t, chosen in the inertial frame (0) of the origin, may be regarded as a further set of parameters, which for the sake of uniformity we shall write $x^d = \varphi^{d-9}$ $(d = 10, 11, ...)$, thus including them in the components of (x) . There may be any number of them and they all have the value 0 when $\mathbf{x} = \mathbf{0}$ and $t = 0$, but may otherwise be subjected to *gauge transformations* at the whim of the observer.

In practice it is likely that an observational system should be subject to fields of force other than a gravitational force. At a fixed point on the the surface of the earth the gravitational force is in approximate equilibrium with contact forces which have a short range and are recognized to be electric in origin, but are also influenced by the rotation and other motions of the earth. The inertial system adopted by a particular observer is then slowly changing. The requirement that the observer, or more precisely the inertial system in which observations are made, should be force-free is essential if the laws of physics are to be given their traditional interpretation, and in fact most observers are not affected in any obvious way by electromagnetic or nuclear

forces. The same, however, cannot be said of gravitational forces. Einstein perceived the difficulty in reconciling gravity with his *special* theory of relativity, in which the velocity of one inertial system relative to another was not supposed to change with time, whereas the gravitational acceleration may actually vary from one inertial system to another. He eventually developed a generalization which could be interpreted as a new theory of gravitation. In this generalization he introduced the **Principle of Equivalence**, according to which *the effect of gravity on the motion of a particle is equivalent to that of any other force of the same magnitude.* This was a reasonable inference from Galileo's experiment, which showed that the acceleration of an object in the earth's gravitational field was independent of its mass, and guided Einstein's subsequent identification of the gravitational mass of any object with its inertial mass.

In view of the Principle of Equivalence, it was necessary to suppose that an inertial system of the Principle of Relativity should be free of gravitational force, which is only possible if it is moving freely under gravity. But then one inertial system may be accelerated relative to another, unless the the second system is sufficiently near to the first. In his *general* theory of relativity Einstein therefore sought to formulate the law of gravitation, and other physical laws, in a form independent not only of the velocity but of the acceleration of the inertial system.

The Principles of Relativity and Equivalence depend ultimately on the acceptance by the conscious observer that its perceptions of the external world are different from, but entirely consistent with and in no way less valid than those of other conscious observers. The differences are accounted for by the differences in the parameters of the inertial frames. Even setting aside the problems associated with observation and consciousness, in their detailed application the special and the general theories of relativity have not, of course, relied exclusively on the Principles discussed in this section, and in particular the concept of *action* has continued to play a most important role.

1.2 Action

Up to the beginning of the twentieth century, the universal validity of Newton's laws of motion, and his theory of gravitation, had remained unchallenged, and even today they are recognized as sufficient for the prediction of most terrestrial phenomena. Experiments performed to test the theory of relativity, however, have shown that most features of Newtonian mechanics are at best approximate, and require corrections which can be important where velocities approaching the velocity of light, or very strong gravitational fields are involved. But some features of Newtonian physics have been found to retain their validity, in particular those based on the **Principle of Least Action**.

The action $A = A(\Omega)$ is an observable associated with the material content of some region Ω of space and time, bounded by physical events observable in any inertial system (x). If the region Ω consists of two disjoint regions $\Omega^{(1)}$ and $\Omega^{(2)}$, then

$$A = A^{(1)} + A^{(2)}, \qquad A^{(1)} = A(\Omega^{(1)}), \qquad A^{(2)} = A(\Omega^{(2)}). \tag{1.1}$$

and the action is therefore what is known as an *additive* quantity. This implies that A can be expressed as a four-dimensional integral

$$A = \int_{\Omega} \mathcal{L} d^4x = \int \int_{R(t)} \mathcal{L} d^3x dt, \tag{1.2}$$

where $\int_{R(t)} ... d^3x$ is then the three-dimensional integral over the region of space $R(t)$ contained within Ω at time t, and $\mathcal{L}$ is the Lagrangian density, a function of position and time. In the inertial system (x), L is defined by

$$L = \int_{R(t)} \mathcal{L} d^3x, \tag{1.3}$$

so that A can also be expressed as a one-dimensional integral

$$A(t) = \int L(q_k, \dot{q}_k) dt, \qquad \dot{q}_k = \frac{dq_k}{dt'}, \tag{1.4}$$

where (q_k) is a set of observables that are sufficient to completely specify the state of the system at time t. These observables obviously depend on the time, but also on the parameters (x') of the inertial system of the observer, thus:

$$q_k = q_k(t, x') = q_k(t - t', x'_1, x'_2, x'_3, ...). \tag{1.5}$$

The function $L(q_k, \dot{q}_k)$ is then the *Lagrangian* of the system.

The principle of least action states that *when the observables of the physical system have prescribed values on the boundary of any region of space and time, they vary within the region in such a way that the total action within the region has its minimum value.* To apply this principle, suppose that the $q_k(t, x')$ have prescribed values on the three-dimensional boundary of Ω, and consider a small variation $\delta q_k = \delta q_k(t, x')$ of the q_k under the integral in (1.4); the resulting change δA in the action is given by

$$\delta A = \int_{R(t)} \sum_k (f_k \delta q_k + p_k \delta \dot{q}_k) dt, \qquad f_k = \frac{\partial L}{\partial q_k}, \qquad p_k = \frac{\partial L}{\partial \dot{q}_k}. \tag{1.6}$$

But, as $\delta q_k(t, x')$ must be zero at the limits of integration,

$$\int p_k \delta \dot{q}_k dt = -\int \frac{dp_k}{d\tau} \delta q_k dt,$$

and it follows that

$$\delta A = \int \sum_k (f_k - \frac{dp_k}{d\tau}) \delta q_k dt. \tag{1.7}$$

If A has its minimum value this expression must vanish, and since this is so for any choice of the small quantities δq_k, satisfying the constraints at the boundary, it follows that

$$\frac{dp_k}{dt} = f_k. \tag{1.8}$$

These equations, due to Lagrange, are consistent with Newtonian mechanics, where p_k would be interpreted as a momentum, and f_k as the corresponding force. But they are also consistent with the Principle of Relativity, which simply imposes important restraints on the form of the action and the Lagrangian function, as shown in (1.11) below.

All of the fundamental observables of a system: its energy E, its momentum $\mathbf{K}$, its angular momentum $\mathbf{J}$, its central vector $\mathbf{C}$, and certain other 'charges' $Q_1, Q_2, ...$ (including the electric charge of the system) associated with gauge transformations, *can be defined in terms of the action.* To do this it is sufficient to consider a *small* change in the specifications of the inertial system of the observer, from (x') to $(x' + \delta x)$. If the time t' is changed to $t' + \delta t$, the position from $\mathbf{x}'$ to $\mathbf{x}' + \boldsymbol{\delta}\mathbf{x}$, the orientation from $\mathbf{u}$ to $\mathbf{u} + \boldsymbol{\delta}\mathbf{u}$ and the velocity from $\mathbf{v}$ to $\mathbf{v} + \boldsymbol{\delta}\mathbf{v}$ and the gauge parameters from $(\varphi_1, \varphi_2, ...)$ to $(\varphi_1 + \delta\varphi_1, \varphi_2 + \delta\varphi_2, ...)$, the resultant small change $\delta A = A(x' + \delta x) - A(x')$ in the action $A(t)$ can be expressed in the form

$$\delta A = E\delta t - \mathbf{K} \cdot \boldsymbol{\delta}\mathbf{x} - \mathbf{J} \cdot \boldsymbol{\delta}\mathbf{u} + \mathbf{C} \cdot \boldsymbol{\delta}\mathbf{v} + Q_1 \delta\varphi_1 + Q_2 \delta\varphi_2 + ..., \tag{1.9}$$

an identity which serves to define E, $\mathbf{K}$, $\mathbf{J}$, $\mathbf{C}$ and $(Q_1, Q_2, ...)$. *The energy is thus identified as the generator of translations in time, the momentum as the generator of translations in space, the angular momentum as the generator of rotations, the central vector as the generator of boosts, i.e., changes of velocity, and other observables like electric charge as generators of changes of the associated gauge parameters.* The relation $\mathbf{C} = M\mathbf{X}$ connects the central vector $\mathbf{C}$ of the observed system with its total mass M and the position $\mathbf{X}$ of its centre of mass. The prescribed final value of the $q_k(t, x')$ is unaffected by the change of inertial system, so that $q_k(t + \delta t, x' + \delta x) = q_k(t, x')$. If we write

$$\delta q_k = q_k(t, x' + \delta x) - q_k(t, x'),$$

it follows from (1.4), (1.6) and (1.8) that the corresponding change δA in the action is

$$\delta A = L\delta t + \int \sum_k (p_k \delta q_k + f_k \delta \dot{q}_k) dt$$

$$= L\delta t + \sum_k p_k [q_k(t, x' + \delta x) - q_k(t, x')]$$

$$= L\delta t + \sum_k p_k \left(\frac{\partial q_k}{\partial t'}\delta t - \frac{\partial q_k}{\partial \mathbf{x}}\cdot\boldsymbol{\delta}\mathbf{x} - \frac{\partial q_k}{\partial \mathbf{u}}\cdot\boldsymbol{\delta}\mathbf{u} + \frac{\partial q_k}{\partial \mathbf{v}}\cdot\boldsymbol{\delta}\mathbf{v} + \frac{\partial q_k}{\partial \varphi^1}\delta\varphi_1 + \frac{\partial q_k}{\partial \varphi^2}\delta\varphi_2 + \ldots\right),$$

where, according to (1.5), $\partial q_k/\partial t' = -\dot{q}_k$. By comparison of this result with (1.9) we see that the energy E, momentum $\mathbf{K}$, angular momentum $\mathbf{J}$, central vector $\mathbf{C}$, and the 'charges' Q_1, Q_2, ... of the system are given by

$$E = L - \sum_k p_k\dot{q}_k, \qquad \mathbf{K} = -\sum_k p_k \frac{\partial q_k}{\partial \mathbf{x}}, \qquad \mathbf{J} = -\sum_k p_k \frac{\partial q_k}{\partial \mathbf{u}},$$

$$\mathbf{C} = \sum_k p_k \frac{\partial q_k}{\partial \mathbf{v}}, \qquad Q_1 = \sum_k p_k \frac{\partial q_k}{\partial \varphi^1}, \qquad Q_2 = \sum_k p_k \frac{\partial q_k}{\partial \varphi^2}, \qquad \ldots. \quad (1.10)$$

The changes in the δx_d (including δt) in parameters x_d are independent of one another and of the time. Assuming the Principle of Least Action, Lagrange's equations (1.8) are satisfied, so that $\delta A(t)$ vanishes in (1.7), but the same is not true of δA as defined in (1.9)!

We now invoke the Principle of Relativity, which requires that the laws of physics expressed by (1.8) should be the same in all inertial systems, and this can only be so if the action is an *invariant*, independent of the observer. This means that for any *isolated* system, not subject to external forces, the action within the region Ω cannot depend explicitly on the time t, or any of the other parameters (x); it is unchanged under all types of transformations. Provided that these conditions are satisfied, it follows from (1.10) and the mutual independence of the δx_d that the *fundamental observables of an isolated system are all conserved: they do not depend on the time.*

*This conclusion may be verified directly by differentiation of E, $\mathbf{K}$, ... with respect to the time; in its most general form it was first reached by Emmy Noether.

The invariance of the action also entails that if (x) and (x') are inertial systems for two different observers, and L and L' are the corresponding Lagrangians as defined in (1.3), then

$$dA = Ld\tau = L'd\tau'. \quad (1.11)$$

It follows from (1.1) and (1.10) that if the region $R(t)$ occupied by the system consists of two disjoint regions $R^{(1)}(t)$ and $R^{(2)}(t)$ with fundamental observables $E^{(1)}$, $\mathbf{K}^{(1)}$, $\mathbf{J}^{(1)}$, $\mathbf{C}^{(1)}$, $Q_1^{(1)}$, $Q_2^{(1)}$, ... and $E^{(2)}$, $\mathbf{K}^{(2)}$, $\mathbf{J}^{(2)}$, $\mathbf{C}^{(2)}$, $Q_1^{(2)}$, $Q_2^{(2)}$, ... respectively, then

$$E = E^{(1)} + E^{(2)}, \qquad \mathbf{K} = \mathbf{K}^{(1)} + \mathbf{K}^{(2)}, \qquad \mathbf{J} = \mathbf{J}^{(1)} + \mathbf{J}^{(2)},$$

$$\mathbf{C} = \mathbf{C}^{(1)} + \mathbf{C}^{(2)}, \qquad Q_1 = Q_1^{(1)} + Q_1^{(2)}, \qquad Q_2 = Q_2^{(1)} + Q_2^{(2)}, \qquad \ldots. \quad (1.12)$$

The fundamental observables E, $\mathbf{K}$, $\mathbf{J}$, $\mathbf{C}$, Q_1, Q_2, ... are therefore all additive quantities. This result requires that there there should be no significant interaction between isolated systems occupying the two regions.

The ideas developed in this section are fundamental to much of modern physics, but leave unanswered two important questions: what is action, and why should it have its least value? A simplistic answer is that the minimization of the action distinguishes physical from unphysical processes, but provides no reason why the unphysical processes are excluded. More meaningful answers to these questions must be sought in the theory of information, and the theory of measurement and observation, which are not independent of a theory of consciousness. Unfortunately or fortunately, in these areas the certainty and determinism of classical physics have all but disappeared.

1.3 Information and Probability

The simplest type of observation is of an event that has only two possible results: the answer to a question (yes or no), the direction of a vector in one dimension (right or left, up or down, forward or backward), the position of a switch (on or off) or quite generally the result of the measurement of any two valued observable. The outcome of such an observation can be represented as a binary digit n with two possible values, 0 and 1. Before the observation there is only a probability p that the outcome will be 1, and a corresponding probability $1 - p$ that the outcome will be 0. These probabilities are determined by the information available concerning the observable: if there is no information, $p = \frac{1}{2}$, but if there is complete information, $p = n$. If there is partial information, p is a calculated quantity between 0 and 1, and the validity of the calculation can be assessed by performing a large number of observations with the same information and verifying that the average value of n is near to p. There can be no absolute certainty that this will be so, but repeated failures to verify the calculated value may lead to reassessment of the ideas on which the calculation was based! This process is guided by nothing more than a belief in the consistency of conscious experience.

In a more general context, the observation of an event may have more than two possible results. We shall take the view that, in the process of observation, a physical observable a is *measured* and the result of the observation is then one of a finite or infinite set of possible values $(a_1, a_2, \ldots)$ of a. We shall write

$$a = \sum_r a_r g_r, \quad (1.13)$$

where the summation $\sum_r$ is over all *possible* values of r; the *outcome* of the measurement is to assign the value 0 to all of the g_r except one, which cannot be specified in advance but has the value 1. The g_r are then *idempotents*, or *projections*, satisfying

$$g_r g_s = g_r \delta_{rs}, \qquad \sum_r g_r = 1. \quad (1.14)$$

From (1.13) and (1.14) it follows that

$$ag_s = a_s g_s \tag{1.15}$$

so that a_s is also what is called an *eigenvalue* of a.

We denote the *probability* that the observed value of a is a_r by p_r, and the *expectation value* $\langle a \rangle$ of a is then given by

$$\langle a \rangle = \sum_r a_r p_r, \tag{1.16}$$

where, as can be seen from (1.13), p_r is the expectation value of g_r:

$$p_r = \langle g_r \rangle, \qquad \sum_r p_r = 1. \tag{1.17}$$

The expectation value is a calculated quantity which should approximate to the average value found by repeated measurement of the observable under the same experimental conditions. The *variance* or *uncertainty* Δa in the value of a is defined as the positive square root of the expectation value of $(a - \langle a \rangle)^2$, so that

$$(\Delta a)^2 = \langle (a - \langle a \rangle)^2 \rangle. \tag{1.18}$$

It is an immediate consequence of this definition that $\Delta a = 0$ only if just one eigenvalue a_r of r is possible so that the expectation values of a and a^2 are a_r and a_r^2 respectively, and intuitively there is no information to be gained from the measurement of a.

The information I to be gained from the measurement of the observable a may now be defined as the observable with values $-\log p_r$, thus:

$$I = -\sum_r \log(p_r) g_r. \tag{1.19}$$

There would be a problem in the application of this formula if a probability p_r were zero, so that $\log(p_r)$ was infinite, but this would imply that the measurement of a could not yield the value a_r; we shall therefore always restrict the summation over (1.18) to those values of r which correspond to *possible* values of a_r. Some of the probabilities could be arbitrarily small, but these would not significantly affect the expectation value of I, which is

$$\langle I \rangle = -\sum_r \log(p_r) p_r, \tag{1.20}$$

according to the classical definition by Shannon of information to be gained by observation. It is important to distinguish between information to be gained, which is objective though it certainly depends on the inertial system of the observer, and information actually gained, which is subjective and depends on the awareness of the conscious observer. Information usually means information to be gained.

A *bit* is an observable whose measurement can yield only one of two values, normally 0 and 1; thus, if n is a bit, $n(n-1) = 0$. The information to be gained from the measurement of n may therefore be obtained from an application of (1.19) in which the subscript r takes only the values 1 and 2. If nothing is known about a bit, the information to be gained from measurement of the bit is $\log 2$. Since the result of any measurement can be expressed as a binary number, *all information may be expressed in terms of bits.* To do this for an observable a, all that is necessary is to express a, in suitable units, in terms of a sequence $(n^{(1)}, n^{(2)}, ...)$ of bits $n^{(j)}$, thus:

$$a = \sum_j 2^{j-1} n^{(j)},$$

so that the result a_r of the measurement of a is a binary number with digits $n_r^{(1)}, n_r^{(2)}, ...$, where the j-th digit $n_r^{(j)}$ is the measured value of $n^{(j)}$, and is either 0 or 1. Then, since each bit satisfies $n^{(j)2} = n^{(j)}$, the corresponding projection g_r in (1.19) is the product

$$g_r = \prod_j (-1)^{n_r^{(j)}} (n^{(j)} - n_r^{(j)}).$$

The subscript r may be called the *address* of the bit.

Shannon's classical definition in (1.20) satisfies the fundamental requirements of macroscopic physics. For instance, $\langle I \rangle$ is positive or zero, and is zero only where the result of the measurement of a is certain. For since $\log(p_r) \leq 0$, $I = 0$ only if each of the probabilities p_r has the value 0 or 1, and of course it follows from (1.17) that only one of the p_r can have the value 1. The maximum information to be gained from the measurement of an observable with a finite number R of possible values is $\log R$ when all the p_r have the same value $1/R$. These considerations are all equally applicable in classical and quantum mechanics, though in quantum mechanics the possible values of an observable are often called *eigenvalues.*

If an observation is made of two events and there R' possible results of the first event and R'' of the second, then there are $R = R'R''$ possible results of the observation of both events. We shall consider the events as measurements of two different observables a' and a'' with possible values a'_r and a''_s, and write

$$a' = \sum_r a'_r g'_r, \qquad a'' = \sum_s a''_s g''_s, \qquad \sum_r g'_r = \sum_s g''_s = 1, \tag{1.21}$$

where the g'_r and g''_s are projections like the g_r defined in (1.14). The expectation value

$$p_{rs} = \langle g'_r g''_s \rangle = \langle g''_s g'_r \rangle \tag{1.22}$$

is the probability that the r-th possible result of the first measurement *and* the s-th possible result of the second measurement will be observed, while

the expectation values p'_r and p''_s of g'_r and g'_s 'are the probabilities that these results will be observed separately. They therefore satisfy

$$p'_r = \sum_s p_{rs}, \qquad p''_s = \sum_r p_{rs}. \tag{1.23}$$

Also, the *conditional probability* that the s-th result of the second measurement will be observed, when the r-th result of the first measurement has been observed, is

$$p_{(r)s} = p_{rs}/p'_r. \tag{1.24}$$

If the two measurements are *independent* of one another, then $p_{rs} = p'_r p''_s$ and $p_{(r)s} = p''_s$. According to the definition (1.19), the information I' to be gained from the first measurement, and the information I'' to be gained from the second, are

$$I' = -\sum_r \log(p'_r) g'_r, \qquad I'' = -\sum_s \log(p''_s) g''_s, \tag{1.25}$$

whereas the information to be gained from both measurements is

$$I = -\sum_{r,s} \log(p_{rs}) g'_r g''_s. \tag{1.26}$$

*If the two measurements are independent of one another, $I = I' + I''$, so that information to be gained from independent events is additive, like the action, energy or momentum in disjoint regions of space and time. It is of course also true that $\langle I \rangle = \langle I' \rangle + \langle I'' \rangle$.

It is important to notice that the concept of the information to be gained from a measurement does not require that the measurement should actually be performed. The information to be gained from the measurement of the energy and momentum of a macroscopic system, occupying a particular region of space, is therefore a valid concept. In the context of statistical thermodynamics, $\langle I \rangle$ is proportional to but opposite in sign to what has been known, since the nineteenth century, as the *entropy* of a system of this type. There is always a loss of information concerning any system, microscopic or macroscopic, when it interacts with another system, and this loss of information is recognized as equivalent to an increase in the entropy associated with the system. There is a predictable increase with time of the of entropy of a macroscopic system due to irreversible processes, such as viscosity, thermal conduction, diffusion, and chemical and nuclear reactions, and these processes are only absent in dynamical and thermodynamical equilibrium. This is true in particular if the macrosopic system consists of two identifiable subsystems. It should therefore *not* be assumed that measurements performed on two systems which are interacting with one another, or have interacted in the recent past, are independent of one another, though this may be a reasonable approximation for two macroscopic systems in equilibrium with

one another. The information to be gained from the separate measurement of observables of two interacting systems is the same as the information to be gained from a single measurement only when the observables measured are *selected*. We have already seen that the fundamental observables, such as the energy, momentum, angular momentum, and central vector of a *isolated* system, which may consists of two subsystems, are selected in this sense, but there are no others in general.

1.4 Uncertainty and Indeterminacy

We shall now consider some of the circumstances in which the quantal definition of information to be gained as I in (1.19) is necessary to complement Shannon's classical definition as its expectation value $\langle I \rangle$ in (1.20). The quantity $\langle I \rangle$ is a real number, which is featureless and gives no indication of the character of the event that would have to be observed or the nature of the observable a that would have to be measured to gain the information. However, in quantum mechanics the information to be gained depends on what is measured, and this is ensured by the appearance of the projections g_r in the definition (1.19), which in turn guarantees that the information I is uniquely associated with the observable a defined in (1.13). Also, and perhaps more importantly, the information to be gained from the measurement of an observable which is not selected, in the sense already explained, is to some extent unpredictable, and to this extent the measurement results in the discovery or *creation* of new information. The discovery is made not in the act of measurement but by the conscious observer.

The distinction between the information I and its expectation value $\langle I \rangle$ is similar to that made between other observables and their expectation values in statistical physics. There the expectation value $\langle a \rangle$ of an additive microscopic observable a is recognized as the corresponding macroscopic quantity; similarly, the expectation value $\langle \rho \rangle$ of the microscopic density ρ of an additive microscopic observable is recognized as the corresponding macroscopic quantity; and the same applies to electromagnetic field potentials and intensities.

At the microscopic level, the use of quantum mechanics instead of classical mechanics is often necessary. This is implicit in what may be regarded a fundamental theorem of quantum mechanics, first formulated explicitly in what is known as Heisenberg's **Uncertainty Principle**. The word 'uncertainty' is the commonly accepted equivalent of 'Unbestimmtheit' in Heisenberg's original German, but the latter is more accurately translated as 'indeterminacy', since, as Born first pointed out, it is a consequence of quantum mechanics that *the value of a microscopic observable prior to measurement is usually not merely uncertain but indeterminate.*

In quantum mechanics, corresponding to any observable a there is also what is called a complementary observable $\widehat{a}$, and, according to the Uncertainty Principle, the uncertainties Δa and $\Delta\widehat{a}$ in these observables, as defined

in (1.18), satisfy

$$\Delta a \Delta \widehat{a} \geq \tfrac{1}{2}\hbar,$$

$$\hbar = h/2\pi = 1.054588 \times 10^{-27}\text{erg} \cdot \text{sec}^2/\text{s}. \tag{1.27}$$

where h is Planck's constant and $\hbar$ is the microscopic unit of action, also often referred to as Planck's constant. A simple proof of an even more general form of the above inequality will be given later. Here we note the implication that the complementary observables cannot be represented in the same way as a' and a'' in (1.21), where in principle r and s could each have one one possible value and then $\Delta a' = \Delta a'' = 0$. Thus there is no measurement that could determine simultaneously values a_r and $\widehat{a}_s$ for both a and $\widehat{a}$. To provide for this well established fact, we write

$$a = \sum_r a_r g_r, \qquad \widehat{a} = \sum_s \widehat{a}_s \widehat{g}_s \tag{1.28}$$

in the usual way, but, following Born and Jordan, regard the projections g_r and $\widehat{g}_s$ as *matrices* which satisfy the usual relations (1.14), but *do not commute in general.* This means that there are values of r and s such that $g_r \widehat{g}_s \neq \widehat{g}_s g_r$, although $g_r g_s = \delta_{rs} g_r = g_s g_r$ and $\widehat{g}_r \widehat{g}_s = \delta_{rs} \widehat{g}_r = \widehat{g}_s \widehat{g}_r$ for all values of r and s. The proof of the uncertainty relations to be given in Sect. 5.3 makes very effective use of this matrix formulation of quantum mechanics.

The theory of the representation of observables by matrices is given in some detail in the Appendix of this book, but here for convenience we summarize some important ideas which will be needed almost immediately. Any matrix, such as a, is a set of elements, which if denoted by a_{jk} $(j, k = 1, 2, ...)$ can be displayed as a square array with a_{jk} in the j-th row and the k-th column. The *transpose* a^{t} of the matrix a is the matrix with a_{kj} in its j-th row and the k-th column, and is therefore obtained by interchanging the rows and columns of a. The *complex conjugate* a^* of a is the matrix with the complex conjugate a^*_{jk} of a_{jk} in its j-th row and k-th column. The matrix a is said to be *hermitean* if its transpose is the same as its complex conjugate, so that $a_{kj} = a^*_{jk}$. If a is not hermitean, it may still be *pseudo-hermitean*, meaning that there is an hermitean *conjugation matrix* $\bar{c}$, with a square $\bar{c}^2$ equal to the unit matrix, such that $\bar{c}a$ is hermitean. The numbers a_r in (1.28), which represent the possible values of the measurement of the observable a are called *eigenvalues* of the matrix a in quantum mechanics. As the result of the measurement must be a real number, the eigenvalues must be real. In Sect. A.3 it is shown that the eigenvalues of hermitean and pseudo-hermitean matrices are always real, and *under certain conditions* the eigenvalues of real matrices may all also be real. We therefore require that *an observable should be represented by an hermitean matrix, or failing that, by a pseudo-hermitean matrix or by a real matrix of a particular type.* Then there are three types of observable:

(1) hermitean, used almost exclusively in non-relativistic quantum mechanics;

(2) pseudo-hermitean, used particularly in effecting transformations to inertial frames moving relative to the observer; and

(3) real, used particularly in effecting transformations to inertial frames at different places or times.

The third type of observable is of especial interest for several reasons. The transformations connecting the frames of observers at different points of space and time convey geometrical information and in doing so provide a framework for the connection of past events with the present, and prediction of future events as far as that is possible. A primitive observable of the third type is the one essential constituent in the fabrication of geometrically appealing models of structures ranging from elementary particles to the entire universe. The model suggested for an elementary particle is consistent not only with its role in quantized field theory but with a suggested representation in space and time as a *string.* Unlike the classical point particle, a string is pictured as a one-dimensional circular object which in the course of time develops into an approximately cylindrical surface. Surface area of the string is related to the action, and the Principle of Least Action therefore acquires a new meaning in terms of information theory.

In quantum mechanics it remains true that an observable a in suitable units can be expressed in terms of a sequence of commuting bits $n^{(j)}$ $(j = 1, 2, ...)$ of the same type, thus:

$$a = \sum_j 2^{j-1} n^{(j)},$$

and any eigenvalue a_r of a may then be expressed in terms of corresponding eigenvalues $n_r^{(j)}$ of the $n^{(j)}$, which are simply the measured values of the binary digits of a_r of a; however, the bits are themselves quantum-mechanical observables, called *qubits*, and must be represented by matrices. In some applications, the address r of the eigenvalue $n_r^{(j)}$ could itself be the eigenvalue of a quantal observable, but the eigenvalues of both are possible numerical results of observation and are therefore always classical quantities. The simplest observables are those which can be represented by only one qubit; several examples will be given in the following chapter.

The implications of the principles uncertainty and indeterminacy extend to the theory of measurement of physical observables. The quantum theory of information provides a satisfactory account of how the result of the measurement of a microscopic quantity may be obtained from the observation of the change of state of a suitably designed detector. Since the detector is necessarily a macroscopic system, the observation is not different in kind from the observation of any other macroscopic event.

However, the process by which information is actually gained from the measurement depends on the participation of a conscious observer, in whose

absence the functioning of the detector remains uncertain, though not indeterminate. The concept of consciousness was one which for a long time was poorly understood, partly because it was not well defined and partly because the physical mechanism by which the cortex of an animal becomes selectively aware of sensory impressions and initiates voluntary action were unknown. Probably because of an intuition on the part of most humans that their future actions are not completely determined, a consensus has emerged in the literature that the mechanism must be of a quantal, rather than classical nature, and a variety of suggestions have been made concerning the cortical structures that could be sensitive to quantal effects. In the final sections of Chap. 8 it will be argued that the quantal effects are in the microscopic channels that are known to permeate the unmyelinated cells of the grey matter of the cortex. These channels are in an electrostatically metastable state easily affected by very small fluctuations in potential in the extracellular fluid. A theory of consciousness will be outlined that accounts in a physically meaningful way for the objective gain and creation of information by the animate observer. The information is derived from a very wide range of physical phenomena that will be described in some detail in the intermediate chapters.

2. Quantal Bits

In quantum mechanics there are various observables that may be represented by a matrix n with two rows and columns satisfying the relations

$$n^2 = n, \qquad \mathrm{tr}(n) = 1. \tag{2.1}$$

where tr denotes the *trace*, i.e., the sum of the diagonal elements of the matrix. We shall refer to such observables as *quantal bits* or *qubits*. In the future these may play an important role in quantum computing, but in the following we shall give emphasis to the physical applications, which in the present chapter include the construction of simple geometrical models and the representation of creation, annihilation and existence operators of fermions, and of their spin. The numerical solution of the characteristic equation $n(n-1) = 0$ satisfied by n allows only the values 0 and 1, and these are the eigenvalues of the matrix n, and they are the only values that may be obtained by measurement of the observable.

The theory of matrices is developed in some detail in Appendix A. Here we note, firstly, that the number of rows and columns of a square matrix is known as its order or *degree*, which determines the number of eigenvalues of the matrix, and a qubit is therefore represented by a matrix of the second degree. Whatever the degree, if m_{jk} denotes the element in the j-th row and the k-th column of any matrix m, the product of m with a similar matrix n is the matrix mn of the same degree, with elements

$$(mn)_{jk} = \sum_l m_{jl} n_{lk}, \tag{2.2}$$

A matrix n of the second degree has the explicit form

$$n = \begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix},$$

when expressed in terms of its elements n_{jk} $(j, k = 1, 2)$, which are complex numbers in general, and the relations (2.1) can be written

$$\sum_l n_{jl} n_{lk} = n_{jk}, \qquad \sum_l n_{ll} = 1 \qquad (l = 1, 2) \tag{2.3}$$

The determinant of any matrix is the product of its eigenvalues, and for the matrix n this easily verified by setting $j = k = 1$ in the first of of the equations (2.3), thus:

$$\det(n) \equiv n_{11}n_{22} - n_{12}n_{21} = n_{11}(1 - n_{11}) - n_{12}n_{21} = 0. \tag{2.4}$$

We shall make use of certain conjugates, described in Appendix A, of the matrix n. In this context they are

(i) The transpose n^{t} of n with elements $n^{\mathrm{tr}}_{jk} = n_{kj}$, given explicitly by

$$n^{\mathrm{tr}} = \begin{pmatrix} n_{11} & n_{21} \\ n_{12} & n_{22} \end{pmatrix}.$$

If $n^{\mathrm{t}} = n$, n is symmetric.

(ii) The complex conjugate n^* of n, with elements n^*_{jk} which are the complex conjugates of corresponding elements n_{jk} of n. If $n^* = n$, then n is real.

(iii) The hermitean conjugate $n^\dagger$ of n with elements $n^\dagger_{jk} = n^*_{kj}$. If $n^\dagger = n$, then n is hermitean.

(iv) The pseudo-hermitean conjugate $\bar{n} = \bar{\mathrm{c}}n^\dagger\bar{\mathrm{c}}$ of n with respect to an hermitean matrix $\bar{\mathrm{c}}$ satisfying $\bar{\mathrm{c}}^2 = 1$. If $\bar{n} = n$, then $\bar{\mathrm{c}}n$ is hermitean, and n is pseudo-hermitean.

The qubit n is an observable with two projections g_1 and g_2, corresponding to its eigenvalues 0 and 1. The expectation value $p = \langle n\rangle$ of n is the probability that the measurement of n will yield the value 1. Any observable a with just two eigenvalues a_1 and a_2 can be expressed in terms of a bit such as n:

$$a = a_1g_1 + a_2g_2, \qquad g_1 = n, \qquad g_2 = 1 - n. \tag{2.5}$$

In a representation of degree 2 the projections g_1 and g_2 are both qubits, and as $g_1g_2 = 0$, these relations are consistent with (1.13) and (1.14).

If f is any numerical function of a real variable, with finite values $f(a_1)$ and $f(a_2)$, a matrix function $f(a)$ of an the observable a can be defined by

$$f(a) = f(a_1)g_1 + f(a_2)g_2. \tag{2.6}$$

If $p_1 = \langle g_1\rangle$ and and $p_2 = \langle g_2\rangle$ are the probabilities that a measurement of a selected observable a will yield the values a_1 and a_2, respectively, the quantal information to be gained from such a measurement is

$$I = -(\log p_1)g_1 - (\log p_2)g_2, \tag{2.7}$$

while the classical information is its expectation value

$$\langle I\rangle = -(\log p_1)p_1 - (\log p_2)p_2.$$

Solutions of the fundamental equations (2.1) can be obtained *either* in terms of a *vector matrix*, which is a square root of the unit matrix, *or* in terms of a two-dimensional complex vector, called a *spinor*. The spinor solutions have their advantages, but we shall begin by discussing the matrix solutions.

Matrix Solutions. There are three different types of qubits:

(1) The first type of qubit has many applications in physics, in particular to the creation and annihilation of particles such as electrons, and also to their spin, as described in Sects. 2.1 and 2.3 below. A qubit of this type will be denoted by $n(\xi)$ and called *hermitean*; it is represented by a matrix of the type

$$n(\xi) = \begin{pmatrix} \frac{1}{2}(1 - \xi_3) & \frac{1}{2}(\xi_1 - \mathrm{i}\xi_2) \\ \frac{1}{2}(\xi_1 + \mathrm{i}\xi_2) & \frac{1}{2}(1 + \xi_3) \end{pmatrix}, \qquad \xi_1^2 + \xi_2^2 + \xi_3^2 = 1, \tag{2.8}$$

depending on a unit vector $\boldsymbol{\xi}$ with three real cartesian components (ξ_1, ξ_2, ξ_3), restricted to the surface of a sphere of unit radius with its centre at the origin. It may be verified this expression for $n(\xi)$ satisfies the requirements of (2.1) either directly or by writing

$$n(\xi) = \tfrac{1}{2}(1 + \xi), \qquad \xi = \xi_1\sigma_1 + \xi_2\sigma_2 + \xi_3\sigma_3,$$

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_2 = \begin{bmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{bmatrix}, \qquad \sigma_3 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{2.9}$$

where σ_1, σ_2 and σ_3 are called *Pauli matrices*. They satisfy the relations

$$\sigma_1^2 = \sigma_2^2 = 1, \qquad \sigma_1\sigma_2 = -\sigma_2\sigma_1 = \mathrm{i}\sigma_3, \tag{2.10}$$

from which the further relations

$$\sigma_3^2 = 1, \qquad \sigma_2\sigma_3 = -\sigma_3\sigma_2 = \mathrm{i}\sigma_1, \qquad \sigma_3\sigma_1 = -\sigma_1\sigma_3 = \mathrm{i}\sigma_2,$$

obtained by cyclic permutation of the subscripts are easily obtained. They are all hermitean and the associated vector matrix ξ in (2.9) is therefore hermitean.

From these relations it follows that ξ in (2.9) satisfies $\xi^2 = 1$, so that $n^2(\xi) = n(\xi)$; also $\mathrm{tr}[n(\xi)] = \mathrm{tr}(\frac{1}{2}) = 1$. For any matrix a of this type, the transpose of a is $\sigma_1 a\sigma_1$, so the transposition matrix c^{tr} is σ_1.

The matrix $n(-\xi) = 1 - n(\xi)$ obtained by reversing the sign of ξ is also a qubit, called the *complementary* qubit of $n(\xi)$. The coefficents ξ_1, ξ_2 and ξ_3 of the Pauli matrices in (2.9) are real, and in some applications are interpreted as cartesian coordinates of a point on a sphere of unit radius. Then the cartesian coordinates are assumed to be distances measured along a *right-handed* system axes in the rightward, forward and upward directions, respectively, relative to the observer. The substitution of $-\xi$ for ξ is called an *inversion*, and cannot be accomplished by a rotation, but only by a change from a right-handed to a left-handed system of axes. Since ξ_1, ξ_2 and ξ_3 are coordinates of a point on a unit sphere, this type of hermitean qubit may also be called *spherical*.

(2) The next type of qubit, denoted by $n(\omega)$ and called pseudo-hermitean, has important applications to time-like vectors such as the normalized

energy–momentum of a physical system, as described in Sect. 2.4. In this instance we define

$$n(\omega) = \begin{bmatrix} \frac{1}{2}(1-\mathrm{i}\omega_1) & \frac{1}{2}\mathrm{i}(\omega_2+\omega_0) \\ \frac{1}{2}\mathrm{i}(\omega_2-\omega_0) & \frac{1}{2}(1+\mathrm{i}\omega_1) \end{bmatrix} \qquad \omega_0^2-\omega_1^2-\omega_2^2=1, \tag{2.11}$$

where the vector $\boldsymbol{\omega}$ with real cartesian components $(\omega_0,\omega_1,\omega_2)$ is now restricted to a hyperboloid of two sheets. This definition can also be written in the form

$$n(\omega) = \tfrac{1}{2}(1+\omega), \qquad \omega = \omega_0\rho_0-\omega_1\rho_1-\omega_2\rho_2, \tag{2.12}$$

where ρ_0, ρ_1, and ρ_2 are matrices satisfying relations

$$\rho_1\rho_2 = \mathrm{i}\rho_0 = \rho_2\rho_1, \qquad \rho_1^2=\rho_2^2=-1,$$

like σ_2, $-\mathrm{i}\sigma_3$ and $\mathrm{i}\sigma_1$, respectively, in (2.10). The matrix ρ_0 is imaginary and hermitean, but ρ_1 and ρ_2 are imaginary and anti-hermitean. From these relations, which imply $\rho_0^2=1$, it follows that $\omega^2=1$ and $n^2(\omega)=n(\omega)$.

Since $\rho_0\rho_1=-\mathrm{i}\rho_2$ and $\rho_0\rho_2=\mathrm{i}\rho_1$ are hermitean, $\rho_0\omega$ and $\rho_0 n(\omega)$ are hermitean, and this type of qubit is pseudo-hermitean with respect to the matrix ρ_0. The unit vector ω has a time-like component ω_0 which is greater than the spacelike component ω_s with coordinates (ω_1,ω_2), so that this type of qubit may also be called *time-like. The matrix* $\rho_0 n(\omega)/\omega_0$ *represents a qubit of type* (1).

(3) The third type of qubit, denoted by $n(\eta)$ and called *real*, also has important physical applications, such as in the formulation of a geometry of curved space-time, to be described in Sect. 2.5, and of elementary string theory in Sect. 2.6. The real qubit is defined by

$$n(\eta) = \begin{bmatrix} \frac{1}{2}(1-\eta_1) & \frac{1}{2}(\eta_2+\eta_0) \\ \frac{1}{2}(\eta_2-\eta_0) & \frac{1}{2}(1+\eta_1) \end{bmatrix}, \qquad \eta_1^2+\eta_2^2-\eta_0^2=1, \tag{2.13}$$

where the vector $\boldsymbol{\eta}$ with real cartesian components (η_1,η_2,η_0) is restricted to a hyperboloid of *one* sheet. Alternatively, this can be written in the form

$$n(\eta) = \tfrac{1}{2}(1+\eta), \qquad \eta = \eta_1\tau_1+\eta_2\tau_2-\eta_0\tau_0, \tag{2.14}$$

with matrices τ_1, τ_2 and τ_0 satisfying

$$\tau_1^2=\tau_2^2=1, \qquad \tau_0=-\tau_1\tau_2=\tau_2\tau_1,$$

like σ_3, σ_1 and $-\mathrm{i}\sigma_2$ in (2.10), respectively. The matrices τ_1 and τ_2 are real and hermitean, but as $\tau_0^2=-1$, τ_0 is real and anti-hermitean. The unit vector η has a space-like component η_s of η, with coordinates (η_1,η_2), which is greater in magnitude than the the time-like component η_0, so that the vector η and its associated real qubit $n(\eta)$ will also be called *space-like.*

The matrices ξ, ω and η in (2.9), (2.12) and (2.14) satisfy $\xi^2=\omega^2=\eta^2=1$ and will therefore be called *unit vector matrices.* A *scalar product* $\xi\cdot\xi'$ and a *vector product* $\xi\times\xi'$ can be defined for any pair of matrices ξ and ξ' of this type, fully analogous to the scalar and vector products of ordinary cartesian vector algebra, thus:

$$\xi\cdot\xi' = \tfrac{1}{2}(\xi\xi'+\xi'\xi) = \cos\chi,$$
$$\xi\times\xi' = -\tfrac{1}{2}\mathrm{i}(\xi\xi'-\xi'\xi), \tag{2.15}$$

where $\cos\chi$ is a multiple of the unit matrix but $\xi\times\xi'$ is a multiple of a unit vector matrix.. If ξ and ξ' are hermitean (of type 1), χ is identified as the angle between ξ and ξ' but if ξ and ξ' are pseudo-hermitean or real, it is possible that $\cos\chi$ may be greater than 1 and then χ is imaginary. Since

$$(\xi\cdot\xi')^2+(\xi\times\xi')^2 = \tfrac{1}{2}(\xi^2\xi'^2+\xi'^2\xi^2) = 1$$

we have

$$(\xi\times\xi')^2 = \sin^2\chi, \tag{2.16}$$

and though this may be negative if the qubit is pseudo-hermitean or real, $\xi\times\xi'/\sin\chi$ is always a unit vector matrix. We note that

$$\xi\cdot.\xi\times\xi' = \tfrac{1}{2}[\xi(\xi\times\xi')+(\xi\times\xi')\xi] = 0,$$

so that ξ is orthogonal to $\xi\times\xi'$, and similarly ξ' is orthogonal to $\xi\times\xi'$, as in ordinary vector algebra.

Spinor Solutions. For many purposes it is convenient to express a qubit n as the *outer* product of two two-dimensional vectors, which are complex if n is complex. This is indeed possible, since the relations (2.3) are both satisfied when the qubit n and its elements n_{jk} are expressed in the form

$$n = \phi\bar{\phi}, \qquad \bar{\phi}\phi = 1,$$

$$n_{jk} = \phi_j\bar{\phi}_k, \qquad \sum_l \bar{\phi}_l\phi_l = 1. \tag{2.17}$$

on the understanding that $\phi\bar{\phi}$ denotes the outer (tensor) product, but $\bar{\phi}\phi$ denotes the inner (scalar) product. The first vectorial factor (such as ϕ) of a qubit is called a *spinor* and the second (such as $\bar{\phi}$) is called a *cospinor.*

We can easily show that a factorization can be made for any solution of (2.1). Since the determinant $n_{11}n_{22}-n_{12}n_{21}$ of n is zero, the equations (2.17) are all satisfied by

$$\phi_1 = n_{12}/(n_{22})^{\frac{1}{2}}, \qquad \phi_2=\bar{\phi}_2=(n_{22})^{\frac{1}{2}}, \qquad \bar{\phi}_1 = n_{21}/(n_{22})^{\frac{1}{2}}, \tag{2.18}$$

where the sign of the square root can be chosen to make ϕ_2 and $\bar{\phi}_2$, or their real parts, positive. There are other factorizations, and (2.18) is unique only

in respect of the equality of ϕ_2 and $\bar{\phi}_2$. The three different types of solution are distinguished by the nature of the difference $\delta = (\phi_1 - \bar{\phi}_1)\phi_2$ between the elements on the minor diagonal of n. If δ is imaginary and not greater than 2 in magnitude, n is hermitean; if δ is real, n is real; and if δ is imaginary and greater than 2, n is pseudo-hermitean.

Since the qubit $(1-n)$ complementary to n also satisfies (2.1), it is a qubit and, like n in (2.17), can be expressed with its elements in the form

$$n_{\rm c} \equiv 1 - n = \phi_{\rm c}\bar{\phi}_{\rm c}, \qquad \bar{\phi}_{\rm c}\phi_{\rm c} = 1,$$

$$(n_{\rm c})_{jk} = \delta_{jk} - n_{jk} = \phi_{cj}\bar{\phi}_{ck}, \qquad \sum_l \bar{\phi}_{cl}\phi_{cl} = 1. \tag{2.19}$$

Since $n(1-n) = 0$, the spinors ϕ and $\phi_{\rm c}$ must be *orthogonal*:

$$\bar{\phi}\phi_{\rm c} \equiv \sum_l \bar{\phi}_l\phi_{cl} = 0, \qquad \bar{\phi}_{\rm c}\phi \equiv \sum_l \bar{\phi}_{cl}\phi_l = 0. \tag{2.20}$$

These equations are all satisfied by (2.18) and

$$\phi_{\rm c1} = -n_{12}/(n_{11})^{\frac{1}{2}}, \qquad \phi_{\rm c2} = \bar{\phi}_{\rm c2} = (n_{11})^{\frac{1}{2}}, \qquad \bar{\phi}_{\rm c1} = -n_{21}/(n_{11})^{\frac{1}{2}}, \tag{2.21}$$

*The equations can also be satisfied by expressing

$$\phi_1 = (\xi_1 + {\rm i}\xi_2)/[2(1+\xi_3)]^{\frac{1}{2}}, \qquad \phi_2 = [\tfrac{1}{2}(1+\xi_3)]^{\frac{1}{2}},$$

$$\phi_{\rm c1} = (\xi_1 - {\rm i}\xi_2)/[2(1-\xi_3)]^{\frac{1}{2}}, \qquad \phi_{\rm c2} = -[\tfrac{1}{2}(1-\xi_3)]^{\frac{1}{2}}.$$

in terms of a unit vector $\boldsymbol{\xi}$ which is real when n is hermitean, but has two imaginary components ξ_1 and ξ_3 when n is pseudo-hermitean, and one imaginary component ξ_2 when n is real.

2.1 Creation and Annihilation

The simplest application of the qubit is to the theory of the particles called *fermions*. These include all the well known elementary constituents of matter: electrons, protons, neutrons, and quarks at a still more fundamental level. Indeed, the stability of matter, the electronic structure of atoms and the nucleonic structure of nuclei all depend to a large extent on the fact that these particles satisfy Pauli's *exclusion principle*, according to which it is impossible for two fermions of the same kind to occupy the same state, *e.g.*, to have the same spin and momentum. In this respect fermions are distinguished from *bosons*, which include photons and the strongly interacting mesons found originally in cosmic ray showers. The exclusion principle implies that if n is the number of fermions of a particular type and in a particular state, this is an observable whose eigenvalue can only be 0 or 1 and satisfies the

basic requirements (2.1) of a qubit. In this application, the measurement of the number of observable results in a gain of information concerning the *non-existence* or *existence* of a fermion with the specified properties. Many observations result in the detection of a fermion whose existence was not known previously, and the information gained then necessarily includes the information that it had been *created*.

All fermions can be created and annihilated, though to conserve angular momentum it is necessary that another fermion should be created or annihilated in the same event. Thus an electron can be created by a γ-ray in the electrostatic field of a nucleus, but a positron is created in the event, in a process known as *pair production*: $\gamma + \gamma' \rightarrow {\rm e}^- + {\rm e}^+$; in the inverse process, an electron and a positron are annihilated, with the production of γ-rays. Again, in the β-decay of a neutron to a proton, an electron is created together with an anti-neutrino: ${\rm n} \rightarrow {\rm p} + {\rm e}^- + \bar{\rm p}$. When an electron is scattered, it is possible and even advantageous to take the view that the electron is annihilated, and replaced by another with a different momentum.

In this application the qubit n representing a fermion is hermitean; the eigenvalues 0 and 1 of n correspond to physical states in which the non-existence or existence of a specified fermion has been confirmed experimentally at a particular time. To represent the creation and annihilation of a fermion in the specified state, we introduce the *creation and annihilation operators* $\bar{f}$ and f; these are matrices of the same degree as n, with elements

$$\bar{f}_{jk} = \phi_j\bar{\phi}_{ck}, \qquad f_{jk} = \phi_{cj}\bar{\phi}_k, \tag{2.22}$$

where ϕ_j and ϕ_{ck} have the same meaning as in (2.18) and (2.19). They are non-hermitean matrices, though $\bar{f}$ is the hermitean conjugate of f, and satisfy

$$\bar{f}f = n, \qquad f\bar{f} = 1 - n, \qquad f^2 = \bar{f}^2 = 0, \tag{2.23}$$

It follows that $fn = (1-n)f$, so that the eigenvalue of the observable n is changed by f from 1 to 0; also $\bar{f}(1-n) = n\bar{f}$, so that the eigenvalue is changed by $\bar{f}$ from 0 to 1; also $f(1-n) = \bar{f}n = 0$, so that it is impossible to annihilate a fermion of the specified type unless one already exists, or create another if one already exists.

If, as in (2.9), we write $n = \frac{1}{2}(1+\xi)$, the matrix

$$\xi = 2n - 1 \tag{2.24}$$

satisfies $\xi f = -f\xi$ and $\xi\bar{f} = -\bar{f}\xi$ and is therefore said to *anti-commute* with f and $\bar{f}$. In Sect. 4.3 this matrix will be found useful in constructing anti-commuting creation and annihilation operators for fermions of different types, and in Sect. 4.4 it will be shown that creation and annihilation operators for bosons can also be constructed from fermionic constitutents.

2.2 Classical Geometry on a Sphere

Spherical geometry has a special importance in physics, originally perhaps because the surface of the earth approximates to a sphere, and more recently because there is reason to believe that the three-dimensional space which contains the earth is also curved. But the animate observer's perception of the external world is based mainly on the visual information conveyed by the multitude of photons incident on the eye from various sources, each of which can be specified by a unit vector in the direction of incidence, or equivalently a point with real polar angles (θ, φ) on a sphere of unit radius.

The cartesian components (x_1, x_2, x_3) of the unit vector $\mathbf{x}$ drawn from the centre of a sphere of unit radius to a point P on its surface are real variables and can be expressed in terms of the polar angles, thus:

$$x_1 = \sin\theta\cos\varphi, \qquad x_2 = \sin\theta\sin\varphi, \qquad x_3 = \cos\theta, \tag{2.25}$$

where $0 \le \theta \le \pi$ and $0 \le \varphi < 2\pi$; the angle θ is called the *co-latitude* and φ the *longitude*.From the cartesian components we can construct a real matrix x of degree 3 with components $x_{\alpha\beta} = x_\alpha x_\beta$:

$$z = \begin{pmatrix} x_1^2 & x_1x_2 & x_1x_3 \\ x_2x_1 & x_2^2 & x_2x_3 \\ x_3x_1 & x_3x_2 & x_3^2 \end{pmatrix}. \tag{2.26}$$

This matrix suffers from the disadvantage that it cannot distinguish between the vectors $\mathbf{x}$ and $-\mathbf{x}$, or the antipodal points (θ, φ) and $(\pi - \theta, \varphi \pm \pi)$ on a sphere, but it is nevertheless useful for the representation of a small area of the sphere, or even an entire hemisphere.

A matrix of degree 3 does not represent a qubit, but x satisfies the same relations

$$x^2 = x, \qquad \mathrm{tr}(x) = 1 \tag{2.27}$$

as n in (2.1), and when $x = x(\theta, \varphi)$ is used to represent a point, the geometry of the sphere can be developed in terms of such points.

*There are three matrices g_r of degree 3 satisfying (1.14); if $x = g_1$, then x can be expressed in the form $\sum_{r=1}^{3} x_r g_r$, where $x_1 = 1$ and $x_2 = x_3 = 0$; thus, unlike a qubit, x has *two* zero eigenvalues.

A great circle, denoted by $x \vee x'$ and called the *join* of x and x', passes through any two distinct points $x = x(\theta, \varphi)$ and $x' = x(\theta', \varphi')$ on the sphere; this can be represented by the matrix

$$x \vee x' = (x - x')^2/[1 - \mathrm{tr}(xx')]. \tag{2.28}$$

*For finite matrices x and x', $\mathrm{tr}(x'x) = \mathrm{tr}(xx')$, so that $\mathrm{tr}(x \vee x') = 2$.

In general, the trace of a matrix representing a geometrical object is $d+1$, where d is the *physical dimension* of the object. The matrix $x \vee x'$ is projective: $(x \vee x')^2 = x \vee x'$.

A point x'' is said to be on the great circle $x \vee x'$ if $x''(x \vee x') = x''$.

In terms of x and x', the angular separation χ of the points $x(\theta, \varphi)$ and $x(\theta', \varphi')$ is given by $\cos^2\chi = \mathrm{tr}(xx')$, where

$$\cos\chi = x_1x_1' + x_2x_2' + x_3x_3' = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi'). \tag{2.29}$$

2.3 Spin and Rotation

Our next example of a qubit is provided by any of the cartesian components s_α $(\alpha = 1, 2, 3)$ of the *spin* $\mathbf{S}$ of an elementary fermion or any other system of spin $\frac{1}{2}$: these are two-valued observables each of which has the eigenvalues $-\frac{1}{2}\hbar$ and $+\frac{1}{2}\hbar$, in terms of Planck's constant. The spin matrices were introduced historically by Pauli to represent the spin angular momentum of the electron, and are simply related to the Pauli matrices σ_α defined in (2.9), thus:

$$s_\alpha = \tfrac{1}{2}\hbar\sigma_\alpha. \tag{2.30}$$

In more recent practice this definition of the spin angular momentum has been extended to all particles with with spin $\frac{1}{2}$, including protons and neutrons. It was already known from the early days of quantum mechanics that the cartesian components (J_1, J_2, J_3) of the angular momentum $\mathbf{J}$ of any system were observables satisfying the relations

$$J_1J_2 - J_2J_1 = \mathrm{i}\hbar J_3, \qquad J_2J_3 - J_3J_2 = \mathrm{i}\hbar J_1, \qquad J_3J_1 - J_1J_3 = \mathrm{i}\hbar J_2. \tag{2.31}$$

Pauli noticed that, because of the relations (2.10), the matrices s_a satisfy these relations, and the vector $\mathbf{s}$ could therefore represent the angular momentum associated with the spin of the electron, even though this was regarded as a point particle. Today it is convenient to *define* angular momentum, in units of $\hbar$, as the *generator of rotations*, and in this section we shall show that (2.30) is consistent with this definition. If a unit vector in the direction ξ is rotated in the direction ξ', the rotation is determined by the angle χ between ξ and ξ', and the axis of rotation which is in the direction of the vector $\xi \times \xi'$. The rotation may be in physical space, where particles are created and annihilated, or in momentum space where their state of motion is represented.

We first notice that the expression (2.8) for $n(\xi)$ may be satisfied by adopting polar angles (θ, φ), with $0 \le \theta \le \pi$ and $0 \le \varphi < 2\pi$, as coordinates for the point ξ on the unit sphere, so that the qubit $n(\xi)$ has the form

$$n(\xi) = \tfrac{1}{2}(1 + \xi), \qquad \xi = \begin{bmatrix} -\xi_3 & \xi_1 + \mathrm{i}\xi_2 \\ \xi_1 - \mathrm{i}\xi_2 & \xi_3 \end{bmatrix},$$

$$\xi_1 = \sin\theta\cos\varphi, \qquad \xi_2 = \sin\theta\sin\varphi, \qquad \xi_3 = \cos\theta. \tag{2.32}$$

As should be expected from the fact that its eigenvalues are -1 and 1, the determinant of any unit vector matrix ξ is $\det(\xi) = -1$.The angles θ and φ that appear in (2.32), and determine the qubit uniquely, can be interpreted as the polar angles introduced in the last section as parameters of a point P on a sphere. If the sphere is of unit radius, then (ξ_1, ξ_2, ξ_3) are the cartesian coordinates of the same point, relative to an origin at the centre, and with the ξ_3-axis through the pole. These coordinates on the unit sphere satisfy the condition $\xi_1^2 + \xi_2^2 + \xi_3^2 = 1$ of euclidean geometry, corresponding to the fact that the qubit is hermitean (type 1).

We note that $1 - n(\xi) = n(-\xi)$ is the qubit corresponding to the point P_a which is at the *antipodes* of P on the sphere. If the sphere is rotated about a suitable axis through its centre, the qubit $n(\xi)$ may be changed, or *transformed*, to the qubit $n(\xi')$ associated with any other point on the sphere with cartesian coordinates (ξ_1', ξ_2', ξ_3'). We shall show that, corresponding to the fact that $n(\xi)$ is hermitean, the transformation may be effected by a matrix $u(\xi', \xi)$ called a *rotation*, thus:

$$n(\xi') = u(\xi', \xi) n(\xi) u^{-1}(\xi', \xi). \tag{2.33}$$

Since $n(\xi')$ must also be hermitean, the inverse $u^{-1}(\xi', \xi)$ of $u(\xi', \xi)$ must also be its hermitean conjugate:

$$u^{-1}(\xi', \xi) = u^*(\xi', \xi); \tag{2.34}$$

the rotation matrix $u(\xi', \xi)$ is therefore of the type called *unitary*. It is not unique, since any expression for $u(\xi', \xi)$ which satisfies (2.33) can be multiplied on the right by a unitary factor depending on ξ and still satisfy the same equation. We shall therefore seek to construct a *simple* rotation, by requiring also that *it should depend only on the angle and axis of rotation*, determined by the scalar and vector products $\xi \cdot \xi'$ and $\xi \times \xi'$ respectively.

We shall give a construction that makes use of the exponential function, which for a matrix of degree 2 can be defined either as in (2.6), or equivalently by the use of its expression as a power series; thus, for any matrix ξ satisfying $\xi^2 = 1$ and any real or complex value of α,

$$\exp(\mathrm{i}\alpha\xi) = 1 + \mathrm{i}\xi\alpha - \tfrac{1}{2}\alpha^2 - \tfrac{1}{6}\mathrm{i}\xi\alpha^3 + \ldots = \cos\alpha + \mathrm{i}\xi\sin\alpha.$$

In this formula we replace ξ by the unit vector matrix $(\xi \times \xi')/\sin\chi$ which was introduced in (2.15) and (2.16), and set $\alpha = -\frac{1}{2}\chi$, obtaining what we shall show to be the rotation matrix:

$$u(\xi', \xi) = \exp[-\tfrac{1}{2}\mathrm{i}\chi(\xi \times \xi')/\sin\chi] = \cos(\tfrac{1}{2}\chi) - \mathrm{i}\sin(\tfrac{1}{2}\chi)(\xi \times \xi')/\sin\chi. \tag{2.35}$$

The angle χ is given by $\cos\chi = \xi \cdot \xi'$, which is expressed in terms of the polar angles of the two vectors in (2.19).

To verify that (2.35) satisfies (2.33), we note that the inverse of $u(\xi', \xi)$, so defined, is

$$u^{-1}(\xi', \xi) = \exp[\tfrac{1}{2}\mathrm{i}\chi(\xi \times \xi')/\sin\chi] = \cos(\tfrac{1}{2}\chi) + \mathrm{i}\sin(\tfrac{1}{2}\chi)(\xi \times \xi')/\sin\chi.$$

Also, since $\xi \times \xi'$ anticommutes with ξ, i.e., $\xi(\xi \times \xi') = -(\xi \times \xi')\xi$, we have $\xi u^{-1}(\xi', \xi) = u(\xi', \xi)\xi$, and

$$\begin{aligned} u(\xi', \xi)\xi u^{-1}(\xi', \xi) &= u^2(\xi', \xi)\xi = (\cos\chi - \mathrm{i}\xi \times \xi')\xi \\ &= \tfrac{1}{2}(\xi\xi' + \xi'\xi - \xi\xi' + \xi'\xi)\xi = \xi', \end{aligned} \tag{2.36}$$

from which (2.33) follows immediately.

There are three rotations of special importance: those which leave one of the coordinates (ξ_1, ξ_2, ξ_3) of the vector matrix ξ unchanged. If $\xi_3' = \xi_3$ in (2.35), so that $\theta' = \theta$, then

$$\xi = \sigma_3\cos\theta + (\sigma_1\cos\varphi + \sigma_2\sin\varphi)\sin\theta,$$

$$\xi' = \sigma_3\cos\theta + (\sigma_1\cos\varphi' + \sigma_2\sin\varphi')\sin\theta;$$

so that $\xi \cdot \xi' = \cos\chi$ and $\xi \times \xi' = \sigma_3\sin\chi$, where $\chi = \theta - \theta'$. The rotation

$$u(\xi', \xi) = \exp(-\tfrac{1}{2}\mathrm{i}\chi\sigma_3) = \exp(-\mathrm{i}\chi s_3/\hbar), \tag{2.37}$$

is clearly through an angle $\theta - \theta'$ about the ξ_3-axis, and the matrix s_3 is the component of the spin angular momentum defined in (2.21). By cyclic permutation of the subscripts 1, 2 and 3 we infer that if, as in (2.30), $s_\alpha/\hbar = \frac{1}{2}\sigma_\alpha$ $(\alpha = 1, 2, 3)$, the unitary matrix $\exp(-\frac{1}{2}\mathrm{i}\chi s_\alpha/\hbar)$ is associated with a rotation through the same angle about the ξ_α- axis. The matrices s_α are therefore said to *generate* rotations about the coordinate axes, and from (2.35) it can be seen that the matrix

$$\tfrac{1}{2}\xi \times \xi'/\sin\chi = \sum_\alpha (\xi \times \xi'/\sin\chi)_\alpha s_\alpha/\hbar$$

is the generator of the rotation of the most general rotation of this type. *We have thus verified that, for a system of spin $\frac{1}{2}$, the angular momentum in units with $\hbar = 1$ is the generator of rotations.*

2.3.1 The Group of Rotations

A transformation of the type $n \to n' = unu^{-1}$ is called a *similarity transformation*. But in (2.34) we have seen that the inverse u^{-1} of the rotation $u = u(\xi', \xi)$ is also its hermitean conjugate, and u is thus a unitary matrix; the transformation $n \to n' = unu^{-1}$ is therefore also a *unitary transformation*.

*The product of two unitary matrices is unitary, so that the result of effecting two successive unitary transformations $n \to n' = unu^{-1}$ and $n' \to n'' = u'n'u'^{-1}$ is the unitary transformation $n \to n'' = u''nu''^{-1}$, where $u'' = u'u$. However, it does not follow that if u and u' are simple rotations, of the form (2.35), then u'' is a simple rotation.

*Any unitary matrix u of this type satisfies the condition $\det(u) = 1$.

The set of rotations of the type $n \to unu^{-1}$ (where $u^{-1} = u^*$) *has the three fundamental requirements of a* group: (i) it includes the unit element $n \to n$, with $u = 1$; (ii) if $n \to n' = unu^{-1}$ and $n' \to n'' = u'n'u'^{-1}$ are rotations, then, since $(u'u)^{-1} = u^{-1}u'^{-1} = u^*u'^* = (u'u)^*$, $n \to n'' = (u'u)n('u)^{-1}$ is also a rotation; and (iii) if $n \to wnw^{-1}$ is a rotation, then since $w(u'u)w = u(u'w)$ and $[(uu')w]^{-1} = [u(u'w)]^{-1}$, the rotations $n''' \to w(u'u)n[w('u)]^{-1}$ and $n''' \to (wu')un[(wu')u]^{-1}$ are the same. The group is called the *special unitary group in two dimensions*, or $SU(2)$, because it acts on matrices of degree 2. It is special because of the condition $\det(u) = 1$ satisfied by all matrices u belonging to the group. We should note, however, that, as discussed in Appendix A, the imaginary unit i may be represented as an antisymmetric matrix, and then certain unitary transformations are also *orthogonal* transformations. Here the corresponding orthogonal group is $SO(3)$; this is said to be *isomorphic* with $SU(2)$.

The simple rotations about the coordinate axes which result from requiring that one of the group parameters is unchanged form *subgroups* of $SO(2)$ of $SO(3)$.

2.4 Lorentz Transformations

In non-relativistic quantum mechanics, it is usual to assume that an observation, in which the presence of a physical system is detected, is made in the inertial frame of the animate observer. The detection of the system implies the measurement of some observable or observables of the system which are then represented by hermitean matrices. However, in relativistic quantum mechanics the detection of the system may be made in an inertial frame which has a velocity different from that of the observer. Then observables are no longer required to be hermitean, but pseudo-hermitean, in the sense that there exists an hermitean conjugation matrix $\bar{c}$, such that $\bar{c}^2 = 1$, and if a is any observable then $\bar{c}a$ is hermitean. The hermitean component $a_s = \frac{1}{2}(a + a^\dagger)$ of a commutes with $\bar{c}$ ($a_s\bar{c} = \bar{c}a_s$), and will be called *space-like*; the anti-hermitean component $a_t = \frac{1}{2}(a - a^\dagger)$ anti-commutes with $\bar{c}$ ($a_t\bar{c} = -\bar{c}a_t$), and will be called *time-like*.

In this section, the observable n representing a pseudo-hermitean qubit is of degree 2, and the conjugation matrix $\bar{c}$ is a matrix ω_0, also of degree 2. The pseudo-hermitean qubit is classified as time-like, since its time-like component is greater in magnitude than its space-like component. We shall investigate in particular the way in which a qubit of this type depends on the velocity of the observer.

As in (2.12), the pseudo-hermitean qubit is denoted $n(\omega)$, where the point with coordinates $(\omega_0, \omega_1, \omega_2)$ is on a hyperboloid $\omega_0^2 - \omega_1^2 - \omega_2^2 = 1$ of two sheets, distinguished by the sign of ω_0. But one sheet in inaccessible by continuous transformations from the other, and there are therefore *two separate varieties of qubits of this type*, one with $\omega_0 > 0$ and the other with $\omega_0 < 0$. In the physical applications of special interest, those with $\omega_0 > 0$ represent *matter*, and those with $\omega_0 < 0$ represent *anti-matter*. There is an *anti-particle* corresponding to any particle with non-vanishing mass: the anti-particle of an electron is a positron, and the anti-particle of a proton is an anti-proton. Similarly, for any system of particles, there is a corresponding *anti-system*. Thus, corresponding to a hydrogen atom, consisting of a proton and an electron, there is an anti-hydrogen atom, consisting of an anti-proton and a positron. The energy of anti-matter, like that of matter, is always positive. Therefore, if E is an eigenvalue of the energy of a system of mass m, and k_1 and k_2 are eigenvalues of components of its momentum in the plane of its motion (so that $k_3 = 0$),

$$\omega_0 = E/(mc^2), \qquad \omega_1 = k_1/(mc), \qquad \omega_2 = k_2/(mc), \tag{2.38}$$

where c is the velocity of light. But for the corresponding anti-system,

$$\omega_0 = -E/(mc^2), \qquad \omega_1 = -k_1/(mc), \qquad \omega_2 = -k_2/(mc).$$

In the following, we shall restrict attention to ordinary matter, for which (2.38) is applicable, with $\omega_0 \geq 1$; ω_1 and ω_2 are then components of the velocity of the system in the plane of motion. Instead of (2.23), there is then a simple parametrization on can be expressed in terms of hyperbolic and circular functions, thus:

$$n(\omega) = \tfrac{1}{2}(1 + \omega), \qquad \omega = \begin{bmatrix} -\mathrm{i}\omega_1 & \mathrm{i}(\omega_2 + \omega_0) \\ \mathrm{i}(\omega_2 - \omega_0) & \mathrm{i}\omega_1 \end{bmatrix} = \omega_0\rho_0 - \omega_1\rho_1 - \omega_2\rho_2,$$

$$\omega_0 = \cosh\mu, \qquad \omega_1 = \sinh\mu\cos\varphi, \qquad \omega_2 = \sinh\mu\sin\varphi, \tag{2.39}$$

where, according to (2.12), $\rho_1\rho_2 = \mathrm{i}\rho_0$ and $\rho_0^2 = -\rho_1^2 = -\rho_2^2 = 1$. If ω' is another unit vector matrix of the same type as ω, a transformation of the type $\omega \to \omega'$, or $n(\omega) \to n(\omega')$, is known as a *Lorentz transformation*, and the matrix $v(\omega', \omega)$ which effects the transformation

$$n(\omega') = v(\omega', \omega)n(\omega)v^{-1}(\omega', \omega) \tag{2.40}$$

is called a *boost*. The boost $v(\omega', \omega)$ is analogous to the the rotation $u(\xi', \xi)$ in (2.33), and the scalar and vector products of ω and ω' are defined by

$$\omega \cdot \omega' = \tfrac{1}{2}(\omega\omega' + \omega'\omega) = \cosh\lambda,$$

$$\omega \times \omega' = -\tfrac{1}{2}\mathrm{i}(\omega\omega' - \omega'\omega), \tag{2.41}$$

where, since $\omega \cdot \omega'$ is never less than 1, λ is always real. The construction of $v(\omega', \omega)$ is also analogous to the construction of $u(\xi', \xi)$ following (2.35). We note that

$$(\omega \times \omega')^2 = 1 - (\omega \cdot \omega')^2 = -\sinh^2\lambda,$$

so that $\mathrm{i}(\omega \times \omega')/\sinh\lambda$ is a unit vector matrix, and the analogue of (2.35) is

$$v(\omega',\omega) = \exp[-\tfrac{1}{2}\mathrm{i}\lambda(\omega\times\omega')/\sinh\lambda] = \cosh(\tfrac{1}{2}\lambda) - \mathrm{i}\sinh(\tfrac{1}{2}\lambda)(\omega\times\omega')/\sinh\lambda. \tag{2.42}$$

Then the inverse of $v(\omega',\omega)$ is

$$v^{-1}(\omega',\omega) = \exp[\tfrac{1}{2}\mathrm{i}\lambda(\omega\times\omega')/\sinh\lambda] = \cosh(\tfrac{1}{2}\lambda) + \mathrm{i}\sinh(\tfrac{1}{2}\lambda)(\omega\times\omega')/\sinh\lambda,$$

and so

$$v(\omega',\omega)\omega v^{-1}(\omega',\omega) = v^2(\omega',\omega)\omega = [\cosh\lambda - \mathrm{i}(\omega\times\omega')]\omega$$

$$= \tfrac{1}{2}\,(\omega\omega' + \omega'\omega - \omega\omega' + \omega'\omega)\omega = \omega',$$

a relation from which the transformation (2.40) follows immediately as required.

Now we consider the special types of Lorentz transformation in which one of the parameters (μ,φ) in (2.39) remains unchanged.

(a) We first consider the rotation needed to change the unit vector matrix ω with parameters (μ,φ) to $\tilde\omega$ with parameters $(\tilde\mu,\tilde\varphi)$ such that $\tilde\mu = \mu$ and $\tilde\varphi = \varphi'$. According to (2.37), $\tilde\omega_0 = \omega_0$, and the energy of the system is the same in the two inertial frames. The only difference between $\tilde\omega$ and ω is in the direction of the momentum, so that the Lorentz transformation is also a rotation. In terms of the parametrization given in (2.39), the energy is $\cosh\mu$, the magnitude of the momentum is $\sinh\mu$, and the scalar product of the two unit vector matrices is

$$\omega\cdot\tilde\omega = \omega_0^2 - \omega_1\tilde\omega_1 - \omega_2\tilde\omega_2 = \cosh\lambda = 1 + 2\sinh^2\mu\sin^2[\tfrac{1}{2}(\varphi-\varphi')],$$

so that $\sinh(\frac{1}{2}\lambda) = \sinh\mu\sin[\frac{1}{2}(\varphi-\varphi')]$, where $\varphi-\varphi'$ is the angle of rotation.

(b) It remains to consider the Lorentz transformation required to change the unit vector matrix $\tilde\omega$ with parameters $(\tilde\mu,\tilde\varphi) = (\mu,\varphi')$, to ω' with parameters (μ',φ'). Since $\varphi' = \varphi$, the momenta are the same direction, and from (2.31) we have

$$\omega = \rho_0\cosh\mu - \tilde\rho_1\sinh\mu, \qquad \omega' = \rho_0\cosh\mu' - \tilde\rho_1\sinh\mu',$$

where, as $\omega^2 = \omega'^2 = 1$, ρ_0 and $\tilde\rho_1 = \rho_1\cos\varphi + \rho_2\sin\varphi$ must satisfy $\rho_0^2 = -\tilde\rho_1^2 = 1$ and $\rho_0\tilde\rho_1 = -\tilde\rho_1\rho_0$. Thus the scalar and vector products in (2.41) are reduced to

$$\tilde\omega\cdot\omega' = \cosh(\mu-\mu') = \cosh\tilde\lambda,$$

$$\omega\times\omega' = \sinh(\mu-\mu')\tilde\rho_2, \qquad \tilde\rho_2 = i\tilde\rho_1\rho_0 = (\rho_2\cos\varphi - \rho_1\sin\varphi)$$

where $\tilde\rho_2 = -1$, so that $\tilde\lambda = \mu-\mu'$ and the analogue of (2.37) is

$$v(\omega',\tilde\omega) = \exp[-\tfrac{1}{2}\mathrm{i}(\mu-\mu')\tilde\rho_2] = \exp(-\tfrac{1}{2}\tilde\lambda\mathrm{i}\tilde\rho_2).$$

This result shows that $\tilde\rho_2$ is the generator of Lorentz transformations of this type. Also, (2.42) yields $\omega' = \tilde\omega\exp(-\tilde\lambda\mathrm{i}\rho_2)$ and

$$\omega_0' = (1-\beta^2)^{-\frac{1}{2}}(\tilde\omega_0 - \beta\tilde\omega_1), \qquad \omega_1' = (1-\beta^2)^{-\frac{1}{2}}(\tilde\omega_1 - \beta\tilde\omega_0), \qquad \omega_2' = \tilde\omega_2 \tag{2.43}$$

if $\beta = \tanh\tilde\lambda$ and $\cosh\tilde\lambda = (1-\beta^2)^{-\frac{1}{2}}$. These are equivalent to Lorentz's relations connecting the values $m(\tilde\omega_0,\tilde\omega_1)$ and $m(\omega_0',\omega_1')$ of the energy-momenta of a system of mass m, observed in two different inertial frames, one of which is moving with a velocity β (in units of $c = 2.9979246\times10^{10}$, the velocity of light) relative to the other.

A boost such as $v = v(\omega',\tilde\omega)$ will be called *pseudo-unitary*, to correspond with the fact that the qubit is pseudo-hermitean. Like rotations, Lorentz transformations form a group, since if $\omega\to\omega' = v\omega v^{-1}$ and $\omega'\to\omega'' = v'\omega'v'^{-1}$, where $v' = v(\omega'',\omega')$, are Lorentz transformations, then so is $\omega\to v''\omega''v''^{-1}$, where $v'' = v(\omega'',\omega)$, though the boost v'' is usually different from $v'v$. The group of Lorentz of this type is denoted by $SU(1,1)$, to distinguish it from $SU(2)$, but this is not the equivalent of the full Lorentz group which includes both $SU(1,1)$ and $SU(2)$ as subgroups, as will appear in Sect. 3.5. The orthogonal group isomorphic with $SU(1,1)$ is $SO(2,1)$.

2.5 Translations in Space and Time

An even more remarkable physical application of quantal units of information and their transformations is to be found in the properties of real qubits, which will be considered next in this section, and feature the *coordinate representation*. The application is to a subspace of curved space-time with two space-like dimensions and one time-like dimension, and the transformations can then be considered as *translations*, or movements from one point of space-time to another. The theory of relativity theory does in fact allow and predict different rates of progress into the future for observers moving with different velocities, though probably not into the past. However, the quantum theory places limitations on the prediction of future events, since only selected information that can be gained from a measurement of a qubit and new information may be created or discovered in the process of measurement.

The real qubit is denoted by $n(\eta)$, and the point with coordinates (η_1,η_2,η_0) is on the hyperboloid $\eta_1^2+\eta_2^2-\eta_0^2 = 1$ of one sheet, with the parametrization

$$n(\eta) = \tfrac{1}{2}\,(1+\eta), \qquad \eta = \begin{bmatrix} -\eta_1 & \eta_2-\eta_0 \\ \eta_2+\eta_0 & \eta_1 \end{bmatrix} = -\eta_0\tau_0 + \eta_1\tau_1 + \eta_2\tau_2,$$

$$\eta_1 = \sin r\cosh t, \qquad \eta_2 = \cos r\cosh t, \qquad \eta_0 = \sinh t, \tag{2.44}$$

in terms of the real variables r and t, the former replacing the angle φ in (2.39). The τ-matrices are used for the coordinate representation, and satisfy $-\tau_0^2 = \tau_1^2 = \tau_2^2 = 1$.

In geometrical terms, r is a measure of distance, in units of $R \simeq 10^{27}$ cm, and t a measure of time, in units of R/c, in the inertial frame of an observer of the qubit at the point $\eta_0 = \eta_1 = 0$. In the application to space-time, η_1 and η_2 are interpreted as the space-like cartesian coordinates of a point on a great circle of a sphere of radius $\cosh t$, in the inertial frame of a detector of the quantal bit, and η_0 is a time-like coordinate in the same inertial frame. The radius $\cosh t = (\eta_1^2 + \eta_2^2)^{\frac{1}{2}}$ of the great circle obviously increases with η_0, and the increase is almost linear when t is very large. We are thus provided with a $2+1$-dimensional subspace of a model 'universe', which at any particular time is finite in extent but expands with time, in much the same way as the physical universe is believed to do. For very small values of r and t, r approximates closely to the distance from the origin and t to the time, in the specified units, and the great circle approximates closely to a straight line through the origin. At very large distance, there is an horizon at $r = \pi/2$ in the units adopted, which however recedes when it is approached. Other frames of reference, *fully equivalent to the one considered*, are obtained by replacing r and t by $r - r_0$ and $t - t_0$ in (2.44), and have a different horizon, but at the same distance from the observer.

As for other types of qubit, changing $n(\eta)$ to $n(\eta')$ may be effected by a single transformation. The scalar product and vector product of two matrix vectors η and η' associated with qubits of this type are

$$\eta \cdot \eta' = \tfrac{1}{2}(\eta\eta' + \eta'\eta) = \eta_1\eta_1' + \eta_2\eta_2' - \eta_0\eta_0' = \cos\psi,$$

$$\eta \times \eta' = -\tfrac{1}{2}\mathrm{i}(\eta\eta' - \eta'\eta). \tag{2.45}$$

and these expressions are consistent with those given in (2.15). Also, it follows from (2.41) that

$$(\eta \times \eta')^2 = 1 - \cos^2\psi = \sin^2\psi.$$

However, $\eta \cdot \eta'$ may now take any value between $-\infty$ and ∞, so that $\sin\psi$ and therefore ψ may be real *or* imaginary. Also, although η and η' satisfy $\eta^2 = \eta'^2 = 1$, $\eta \times \eta'$ is not always hermitean and its square may be positive or negative. However, $(\eta \times \eta')/\sin\psi$ is always a unit vector matrix.

When ψ is real the transformation of $n(\eta)$ to $n(\eta')$ is a rotation, but one which in the curved space-time has the effect of changing the distance r from the origin, and is therefore characterized as a *translation in space*, in the inertial frame of an observer at the origin. If η_0 is unchanged by the transformation, this is the only effect, but otherwise it changes the time t, and therefore involves a *translation in time*, into the past or future of an observer in the inertial frame of the origin. The translations form a group, which in the present context is denoted by $Sl(2,r)$ when considered as real, or $SO(2,1)$ when considered as pseudo-orthogonal.

The analogue of $u(\xi',\xi)$ in (2.35) is the matrix

$$v(\eta',\eta) = \exp[-\tfrac{1}{2}\mathrm{i}\psi(\eta \times \eta')/\sin\psi] \tag{2.46}$$

and, since, as can be seen from (2.45), η anticommutes with $\eta \times \eta'$, so that

$$v(\eta',\eta)\eta v^{-1}(\eta',\eta) = v^2(\eta',\eta)\eta = \eta[\cos\psi - \mathrm{i}(\eta \times \eta')]$$

$$= \tfrac{1}{2}(\eta\eta' + \eta'\eta - \eta\eta' + \eta'\eta)\eta = \eta'.$$

Since the translation effected by $v(\eta',\eta)$ is in general a Lorentz transformation, and not simply a rotation, it is similar in some respects to the transformations introduced in the last section: it is pseudo-unitary, corresponding to the fact that the qubits are real but not hermitean. Again translations of the type presently considered form a group.

For small changes $d\eta$ of the vector matrix η of a point P, the condition $\eta^2 = 1$ yields $\eta \cdot d\eta = 0$ to the first order of small quantities, and $d\eta^2 = 0$ to second order. If η_α are cartesian coordinates on the hyperboloid, these conditions become

$$\eta_1^2 + \eta_2^2 = \eta_0^2 + 1, \qquad \eta_1 d\eta_1 + \eta_2 d\eta_2 = \eta_0 d\eta_0, \qquad d\eta_1^2 + d\eta_2^2 = d\eta_0^2. \tag{2.47}$$

In the context of the special theory of relativity, which is a very good approximation near the origin at $r = t = 0$, $\eta_1 \simeq r$ is naturally interpreted as the distance from the origin along the η_1-axis, and $\eta_0 \simeq t$ as the time in units such that the velocity of light c is unity. In this approximation, $\eta_2 \simeq 1 + \frac{1}{2}(t^2 - r^2)$ is very near to 1 and is a *Lorentz invariant*, unaffected by changes of orientation and velocity of an observer at the origin. If $t > r$, $\tau = (t^2 - r^2)^{\frac{1}{2}}$ is the *interval* between events the at the origin and the point (r,t), while if $r > t$, $\sigma = (r^2 - t^2)^{\frac{1}{2}}$ is the *separation*. The interval and separation are both zero on the *light cone* $r = t$.

In the more general context when r and t are not small, to investigate the effect of the velocity of the observer on an event observed from the origin, we set $\eta_2' = \eta_2$ in the above, The Lorentz transformation associated with $v(\eta',\eta)$ then has the effect $\eta \to \eta'$, where

$$\eta_0' = (1-\beta^2)^{-\frac{1}{2}}(\eta_0 - \beta\eta_1), \qquad \eta_1' = (1-\beta^2)^{-\frac{1}{2}}(\eta_1 - \beta\eta_0), \qquad \eta_2' = \eta_2, \tag{2.48}$$

and β is the velocity of an inertial frame passing through a point P at distance r from the origin at time t, relative to another passing through the point P′ at distance r' from the origin at time t'. We infer that, in a relativistic theory, the relative velocity of P relative to P′ is not simply $\eta_1/\eta_0 - \eta_1'/\eta_0'$, but

$$\beta = (\eta_1/\eta_0 - \eta_1'/\eta_0')/[1 - \eta_1'\eta_1/(\eta_0'\eta_0)].$$

From this result and (2.44) it can be seen that the velocity of the inertial frame of P relative to the origin is $\eta_1/\eta_0 = \sin r/\tanh t$, when $\eta_2 = \cos r \cosh t$ is invariant, and reduces to r/t only when r and t are small.

We have interpreted r and t as coordinates in physical space, which is very different from the normalized energy–momentum space of the last section. The Lorentz transformation (2.48) is interpreted as showing the effect of a

change of velocity β (in units with c = 1) on the distance and time travelled from the origin in a new inertial frame, instead of the effect on the energy and momentum as in (2.43). But this merely reflects one of the differences between the coordinate representation and the momentum representation and the matrix $v(\eta', \eta)$ effecting the change of velocity may again described as a *boost*.

Finally, we consider the special transformations in which $\eta_0 = \eta'_0 = 0$; although in a curved space-time they are translations in space they may be also be regarded as pure rotations. According to (2.44) and (2.45),

$$\eta \cdot \eta' = \cos(r - r'), \qquad \eta \times \eta' = -\mathrm{i}\sin(r - r'),$$

so that $\psi = r - r'$ and the generator of the rotations is defined as

$$l = -\tfrac{1}{2}\mathrm{i}\hbar\tau_0. \tag{2.49}$$

Unlike the generators introduced in (2.30) identified as spin agular momentum, this generator induces actual orbital motion and is therefore associated with *orbital angular momentum*. In the extension to four-dimensional space-time to appear in later chapters it becomes a three-dimensional vector l.

2.6 Elementary String Theory

Throughout much of the development of classical physics, particles were considered to be moving points. The concept of the smallest part of any object as a point was transferred to elementary particles such as the electron and the photon after their discovery, and survived the discovery of quantum mechanics, even though it became clear that, in the light of Heisenberg's uncertainty principle, that the 'observables' representing the coordinates of a particle could never be measured exactly, and that the position of an unconstrained particle with a precise momentum was completely indeterminate. In principle, the waves associated with such objects in Schrödinger's wave mechanics could fill the entire universe. Bohr, who played an important part not only in the initial theoretical development of atomic physics but in the subsequent interpretation of quantum mechanics, advocated the concept of a *dual* point-like and wavelike nature of the elementary particles, which may be seen as a compromise between the classical and wave-mechanical points of view. In the second half of the twentieth century this somewhat difficult idea was partially eclipsed, in the context of quantized field theory, by Feynman's invention of diagrams in which particles followed well-defined though indeterminate trajectories, thus encouraging and giving new life to the intuitively attractive classical concept of a particle as a moving point.

However, at a time when 'theories of everything' based on quantized field theory appeared to be reaching a mathematical impasse, the development of

string theory has provided a new approach. In string theory, the elementary particle at a particular time is a two-dimensional circular object which in the course of time develops into an open string. There may also be closed strings, which in space-time resemble a torus, but since these are only observable through their interactions with open strings, they can be ignored.

Locally, a string may be pictured as a cylindrical space-time object which in principle could extend to infinity in time in both directions. However, from the point of view of quantal information theory, the simplest model is a qubit of the real type considered in this section. We have already seen that, although in the frame of an observer at the origin the radius of the hyperboloid of one sheet appears to increase in cosmological time, there is no difference between the perceptions of observers in different inertial time frames, and in any local frame the hyperboloid approximates to a cylinder of the same radius. The coordinates of a point on the string may be chosen to be (η_0, η_1), where η_0 is a measure of the time, and η_1 of the distance from the origin in the units adopted. The variables η_0 and η_1 will therefore be used instead of t and x in an application of the theory of least action leading to (1.9).

One of the most striking innovations of string theory is the geometrical interpretation given to the action. According to the theory initiated by Nambu and Goto, the action associated with an isolated string in any region of space time is defined as the negative of its invariant surface area, in appropriate units. The third variable η_2 has been identified as an invariant, and in string theory it is a measure of the invariant surface area. This variable is therefore also a measure of the action, but to represent physical as distinct from unphysical motions must be expressed, as shown in (2.47), in terms of the independent variables η_0 and η_1. From the information-theoretical point of view, *the physical motions selected by the Principle of Least Action are revealed by (2.44) as a transparent consequence of the requirement that the eigenvalues of a real qubit should be 0 and 1.*

In the small rectangular region included between (η_0, η_1) and $(\eta_0 + d\eta_0, \eta_1 + d\eta_1)$ the invariant surface area is $-m(d\eta_0^2 - d\eta_1^2)^{\frac{1}{2}}$, or $-md\eta_2$ in terms of the invariant η_2. In units of $2\pi/m$, the action between the times 0 and η_0 accordingly has the value

$$A = -m\int_0^{\eta_0} [1 - (d\eta_1/d\eta_0)^2]^{\frac{1}{2}} d\eta_0, \tag{2.50}$$

corresponding to a Lagrangian function $m[1 - (d\eta_1/d\eta_0)^2]^{\frac{1}{2}}$. The application of the Principle of Least Action then leads to the expressions

$$k = m(d\eta_1/d\eta_0)[1 - (d\eta_1/d\eta_0)^2]^{-\frac{1}{2}}, \qquad E = m[1 - (d\eta_1/d\eta_0)^2]^{-\frac{1}{2}} \tag{2.51}$$

connecting the eigenvalues of the momentum k and energy E with the velocity $d\eta_1/d\eta_0$. These reduce to well known special relativistic formulas for a particle when η_1 and η_0 are approximated by r and t. As a further important result,

we obtain the special relativistic relation $E^2 = k^2 + m^2$ ($E^2/c^2 = k^2 + m^2c^2$ in units with $c \neq 1$) between the energy, momentum and mass of an isolated particle.

In the fully quantized theory to be developed in subsequent chapters, the action, momentum and energy are fundamental observables and represented by matrices rather than their eigenvalues. However, for an isolated particle the relations connecting these observables are identical with those derived above, and the real qubit is thus qualified as an essential *constituent* of, though certainly not the whole of the information to be gained from the observation of an elementary particle. In the primitive model provided by a single qubit, the radius R of the two-dimensional string would most naturally be expected to be very small. But a comparison of this and the previous section shows that a single string could serve as a model for the whole universe, and the question of size arises only when interactions between different strings are considered. For this purpose we shall require more than one qubit to represent even a single particle, and embedding spaces of more than two dimensions will need to be considered.

2.7 Summary

Information concerning the universe of physics is coded in terms of bits which have observable values 0 and 1. Following the recognition of quantum mechanics as the fundamental discipline of physics, it has become evident that all physical information may be correctly represented in terms of quantal bits, or qubits; these are observables that in the absence of measurement are uncertain or indeterminate, and acquire a definite value 0 or 1 only in the process of observation, which normally requires not only some kind of detector or measuring device, but the participation of a conscious observer who becomes aware of the outcome of the observation through selection mediated by the senses. There are three different types of qubit: the hermitean qubit, which provides the normal representation of information in ordinary quantum mechanics, where the inertial frame of reference is that of the observer, the pseudo-hermitan qubit, adapted to the representation of information derived from other inertial frames, and the real qubit that is appropriate for the representation of information derived from distant sources or cosmological information.

This chapter has been devoted to examples of various types information capable of representation by a single qubit. The first concerns the information to be obtained by observation of the existence or non-existence of a fermion, one of the elementary consitutents of matter of which there can be no more than one of a particular type. This is followed by a simple application to spherical geometry, which in the following chapter will be generalized for the more comprehensive projective geometries that are able to provide more realistic models of space-time. The example given of a pseudo-hermitean qubit

provides an account of the local Lorentz transformations connecting observations in inertial frames not necessarily at rest relative to the observer, though restricted to a projective subspace with one time-like and one space-like dimension. The real qubit has interesting properties that mirror those of a subspace of the de Sitter model of the universe which takes no account of gravity but otherwise provides what is a simple representation of the curvature of space-time. There is also an application, within the limitations of cosmology and the special theory of relativity, to the theory of strings, which has been suggested as an alternative to elementary particle physics as a description of the fundamental constituents of matter.

3. Events in Space and Time

Our understanding of physical space has its historical origin in the system of geometry developed by Euclid. This was based on a collection of axioms and postulates, most of them rather directly related to our primitive perception of physical space. On the basis of the axioms and postulates, a rich variety of theorems could be deduced which could then be confirmed, at least in some approximation, by direct measurement. Only one of the postulates, Euclid's *fifth postulate*, was by no means obvious in its application to physical space. This stated that, given a straight line in a plane, one and only one straight line could be found in the same plane which passed through some point not on the line but did not meet the given line at any finite distance, i.e., was parallel to the given line. The fifth postulate was needed to prove Pythagoras' theorem, and all the relations based on it connecting the distances between points in two or three dimensions.

Euclidean geometry had a profound influence on physics, especially following the introduction by Descartes of a pair of coordinates (x, y) to represent the position of a point in a plane, or a set of three coordinates (x_1, x_2, x_3) to represent the position of a point in three dimensions.Coordinate geometry undoubtedly made an important contribution to Newton's extremely fruitful though ultimately imperfect formulation of the laws of mechanics and gravitation. In the nineteenth and twentieth centuries, it was found very useful to formulate all the laws of physics in terms of scalars, spinors, vectors and tensors with components all of which transform in a particular way under changes of coordinates. Throughout physics it became usual to think of any measurable quantity as a real number, which was either a scalar or a component of a spinor, vector or tensor.

But modern physics is based partly on the theory of relativity, which is concerned primarily with the geometry of space and time, and partly on quantum mechanics, which is concerned with the properties of matter at the most fundamental level.

The theory of relativity was the earliest important revision of the ideas of space and time that formed the basis of Newtonian mechanics. For Newton, time was a numerical property of any event, depending only on the choice of origin (time zero) and the units in which it was measured. The first doubts about this Newtonian concept followed the well known experiments

of Michelson and Morley. in the nineteenth century showing that the velocity of light was not affected by the motion of the earth. This raised serious questions about the ethereal concept of physical space which was then generally accepted, and gradually led to a recognition of the universal validity of the Principle of Relativity: "The laws of physics are the same for all force-free observers, irrespective of their time, position, orientation and state of motion".

This principle had indeed been a feature, though widely unrecognized, of Newtonian physics, and no essential difficulties arose from its application until after the discovery and formulation of the laws of electromagnetism by Faraday and Maxwell in the nineteenth century. Maxwell had found that, according to his formulation, the velocity of propagation of electromagnetic waves in a vacuum was the same as the velocity of light, and reached the marvellous conclusion that light was an electromagnetic phenomenon. The idea was that the light emitted by a source consisted of electromagnetic waves within a certain range of frequencies, corresponding to the visible part of the spectrum. However, the velocity of an ordinary wave is relative to the medium in which it propagates, and the concept of an 'ether' was invented as the medium of propagation of electromagnetic waves. This ethereal concept became untenable following the discovery of Michelson and Morley that the velocity of light appeared to be independent of both the velocity of its source and the means of detection. The natural conclusion was that the velocity of light, c, did not depend on the velocity of the observer.

However, it was not until around the beginning of the twentieth century that the pertinent questions were answered with the development of the special theory of relativity by Einstein, which incorporated the physical perception of Poincaré and mathematical formulation of Lorentz, but also included the important insight that all information concerning the geometry of the physical world depended on the transmission of signals, and especially the transmission of light signals, from one point to another. The result was to overturn the Newtonian concept of the independence of space and time and to inaugurate a new formulation of physics.

Newtonian physics had in fact been based on two questionable postulates. It assumed that, when the units of length and time were fixed,

(i) the time between any two events was a physical *invariant*, independent of the frame of reference adopted by an observer; but also

(ii) the distance between any two *simultaneous* events was also a physical invariant.

This second postulate, through its notion of simultaneity, assumed the validity of the first. Together, they implied that the velocity of light measured in a frame moving in the same direction as a flash of light should be less than that measured in a frame moving in the opposite direction, contrary to the findings of Michelson–Morley experiment.

The most innovative feature of the special theory of relativity was its implication that the space and time of classical physics were not independent of the state of motion of the observer and should be regarded as different aspects of a single four-dimensional *space-time*. An inertial frame was determined in general not simply by the origin of coordinates and the coordinate axes, but also by the velocity of the frame relative to a particular force-free observer. In one inertial frame, the position of an event x in space-time was fixed by the time x^0 of the event, in suitable units, together with the three cartesian coordinates x^1, x^2 and x^3 specifying its position in that frame. For any two such events x and x', instead of the postulates (i) and (ii) above, Einstein assumed that the *separation* σ, or the *interval* τ between the events, defined by

$$\sigma^2 = -\tau^2 = -(x^0 - x'^0)^2 + (x^1 - x'^1)^2 + (x^2 - x'^2)^2 + (x^3 - x'^3)^2$$

was the only physical invariant connecting them, independent not only of the choice of the origin and orientation of the coordinates but also of the velocity of the frame of reference. The unit of the time was chosen so that the velocity of light was 1, so that the separation σ of two events x and x' coinciding with the emission and absorption of a flash of light, was zero; moreover, since σ was independent of the frame of reference, the velocity of the flash of light would be 1 also in any other frame. Einstein's postulate, unlike the Newtonian postulates, was therefore consistent with results of the Michleson-Morley experiment.

It is obviously possible for σ^2 to be negative, if $(x^0 - x'^0)$ is greater in magnitude than the distance between the events; then σ is imaginary but the interval τ is real and is said to be *time-like*. On the other hand, if σ^2 is positive, the separation is real and is said to be *space-like*. A time-like interval between two events can be interpreted as the minimum time required for an observer to travel from one event to the other, and for this reason the interval is often referred to as the *proper time* for light to travel at uniform speed between the events. Time-like and space-like intervals are separated by *light-like* intervals, corresponding to the value $\sigma = 0$. The time required for an observer to reach a distant point of space of course decreases with the speed of travel, but if it were possible for the observer to travel with the speed of light, a distant point of space could be reached in no time at all!

It is usual to introduce *covariant* coordinates, in the most useful notation, by writing

$$x_0 = -x^0, \qquad x_1 = x^1, \qquad x_2 = x^2, \qquad x_3 = x^3,$$

when (x^1, x^2, x^3) are the cartesian coordinates, and similarly for the event x', so that the expression for the separation σ, or the interval τ, may be written

$$\sigma^2 = -\tau^2 = \sum_{\lambda=0}^{3} (x_\lambda - x'_\lambda)(x^\lambda - x'^\lambda). \tag{3.1}$$

Following Einstein's convention, the summation over a repeated affix like λ in an invariant expression is often omitted.

The special theory of relativity implied that space was 'flat' and infinite in all directions, and was therefore inconsistent with our present perceptions of space on the astronomical scale. It is now generally accepted that physical space, like the earth's surface, is not 'flat', but curved, as required by Einstein's general theory of relativity and his theory of gravitation. Quite apart from this, it has gradually been recognized since the work of Desargues in the seventeenth century that the methods of *projective* geometry were very much more powerful than Euclid's. We have seen in the previous chapter how to formulate the Euclidean geometry of the sphere as a two-dimensional projective geometry, and the general theory of relativity led to further applications of this type. Most important of these was de Sitter's model, which represented the entire universe as a four-dimensional hypersphere of constant curvature. De Sitter's model was of great interest because it was able to account in the simplest possible way for the apparent expansion of the universe implied by Hubble's discovery of the recession of distant galaxies. It has been found to be related to a variety of other cosmological models by a simple change of coordinates. Moreover, it is also applicable to smaller regions of space and time where the curvature of space and time attributed to gravitation is practically constant. This model will be discussed in more detail in Sects. 3.1 and 3.2 below.

At least initially, the development of quantum mechanics in the 1920's had little impact on the geometrical basis of physics. The concept of space as a set of points with numerical coordinates survived Heisenberg's discovery that it was impossible to attach any precise numerical meaning to coordinates of elementary particles such as electrons or photons, because they cannot be measured with an arbitrary degree of precision. In 1925 it was first proposed by Born and Jordan that the coordinates of such particles should be represented by *matrices* rather than numbers, and that is the point of view that will be adopted in the following. There can be no reasonable objection to introducing numerical coordinates (x^1, x^2, x^3) to represent the position of the centre of mass of a macroscopic object, such as a measuring device, and a numerical time x^0 or t to represent the time at which a measurement is made. Even in that application, however, there are conceptual advantages in the use of matrices, instead of coordinates, and to begin this chapter we shall present a matrix formulation of projective geometries, including the geometry of de Sitter space.

But these are essentially classical geometries. In quantum mechanics, the emphasis is on the microscopic events involving the creation and annihilation of particles which carry information from one point of space and time to another. The qubit is the fundamental unit of information and we have already seen, in the last chapter, examples of how the creation and annihilation of a single fermion and its spin, as well as some fundamental subspaces of physical space-time can be described in terms of these units. In this chapter we shall go on to examine the different ways in which a pair of qubits can be combined. By these means we shall obtain a complete representation of states of a fermion in the coordinate and momentum representations, and also the spin angular momentum of particles of spin one.

3.1 Projective Geometries

Two-dimensional spherical geometry, as formulated in Sect. 2.3 is a particular example of a projective geometry, where the projection of any point is along the radius vector onto a three-dimensional sphere. De Sitter space provides another example of a classical projective geometry in four dimensions, with one-dimensional subspaces which are time-like and infinite in extent, and three-dimensional curved subspaces with a finite radius R. When R becomes very large, any local region of de Sitter space is indistinguishable from the space-time of special relativity, and any local region of the finite three-dimensional subspaces is indistinguishable from Euclidean space. From this point of view, de Sitter space contains all of the classical spaces of physical significance, with the exception of the Riemannian spaces of the general theory of relativity. Even the latter, however, can be embedded in projective spaces of higher dimensions, and we shall make effective use of this in our presentation of the theory of gravitation in Chap. 7. In the following, we shall therefore consider classical projective spaces in any number of dimensions, and shall represent the spaces and subspaces, including points, by matrices. We note in advance that the degree of the matrix necessary to represent a projective space is always greater by unity than the dimension of the space.

The guiding principles are:

(1) The entire projective space, called the *universe*, is represented by, and thus identified, with the unit matrix 1.

(2) A subspace of the universe is identified with a matrix r satisfying the projective condition $r^2 = r$; this matrix is also required to be *pseudo-symmetric*, meaning that there is a symmetric square root η of the unit matrix, independent of r, such that ηr is symmetric. This condition is obviously the analogue for real matrices of the pseudo-hermitean condition of (2.4). If the subspace r is symmetric, it is space-like; if it is anti-symmetric, it is time-like. The matrix η determines the *metric* of the projective space, and its elements η_{jk} form what is often called the *metric tensor* of the space, though we should note that this term is also applied to $g_{jk} = -\eta_{jk}$.

(3) If the subspaces r and s satisfy $rs = sr = s$, then s is contained in r; but if $rs = sr = 0$ they are disjoint in the sense that one is just over the horizon of the other. As an example of this condition, points on the equator of the unit sphere are disjoint with the poles.

(4) The dimension of a subspace r is $\mathrm{tr}(r) - 1$. In a universe of n dimensions, the *complement* of r is the subspace $1 - r$, which is obviously disjoint

with r; if r is m_r-dimensional, then $1-r$ is $(n-m_r)$-dimensional. The complement of the universe is the particular subspace 0, called *empty* subspace: it does not contain any point.

(5) A point, which here will be represented by a matrix x (or x' or x'', to represent more than one point), is a zero-dimensional subspace, so that $\mathrm{tr}(x)=1$; like x in (2.26) and (2.27), it therefore has only one non-vanishing eigenvalue and the elements of the symmetric matrix x are of the form $x_{jk}=x_jx_k$, where $x_k=\sum_j x^j\eta_{jk}$, so that $\sum_j x_jx^j=1$. We may therefore express x as the outer product $x\bar{x}$ of the vector x with contravariant components x^j and $\bar{x}=xh$ with covariant components x_j, normalized so that their inner product $\bar{x}x=1$. It follows that if r is any subspace, $\bar{x}rx=(\bar{x}rx)x=\mathrm{tr}(rx)x$. Also, if x and x' are points, $\mathrm{tr}(xx')=(\bar{x}x')(\bar{x}'x)=(\bar{x}x')^2$.

(6) The separation $\sigma_{z'z}$ of two points z and z' is given by ${\sigma_{z'z}}^2=\mathrm{tr}[(x'-x)^2]=2-2\mathrm{tr}(x'x)$. If $\sigma^2_{z'z}>0$, the separation is space-like; if $\sigma^2_{x'x}=0$, it is light-like; and if $\sigma^2_{x'x}=-\tau^2_{x'x}<0$, so that $\sigma_{x'x}$ is imaginary but $\tau_{x'x}$ is real, it is time-like; then $\tau_{x'x}$ is the interval between the points. More generally we may define the separation σ_{rs} of two subspaces r and s by

$$\sigma^2_{rs}=\mathrm{tr}[(r-s)^2]. \tag{3.2}$$

These principles serve to establish a precise correspondence between the fundamental notions of classical projective geometry and a set of real matrices. According to (2), any subspace of the universe is represented by a projective pseudo-symmetric matrix r, so that, more formally, we assume that if η is the metric matrix, then

$$r^2=r,\qquad r^{\mathrm{t}}=\eta r\eta,\qquad \eta^{\mathrm{t}}=\eta,\qquad \eta^2=1. \tag{3.3}$$

It follows that r has symmetric and anti-symmetric components $r_s=\frac{1}{2}(r+\eta r\eta)$ and $r_t=\frac{1}{2}(r-\eta r\eta)$, called space-like and time-like components respectively; they are not subspaces, unless one of them vanishes. The unit matrix 1, which represents the entire universe, and the zero matrix 0, which represents the empty subspace, satisfy these conditions in a trivial way.

It is possible, with certain important exceptions, to construct from two projective subspaces r and s two other subspaces $r\vee s$ and $r\wedge s$, called the *join* and the *meet* of r and s, which are of major geometrical importance. The meet will be defined as the complement of the join of the complements of r and s:

$$r\wedge s=1-(1-r)\vee(1-s);$$

and is therefore not an independent concept. The join is the smallest subspace which contains both r and s: $r(r\vee s)=r$ and $s(r\vee s)=s$.; the meet, however, is the greatest subspace contained in both r and s: $r(r\wedge s)=r\wedge s$ and $s(r\wedge s)=r\wedge s$. The dimension of the join is greater by 1 than the sum of the dimensions of the joined subspaces. If r and s are disjoint, their join is $r\vee s=r+s$. More generally, we may suppose that the subspace s is formed

by joining points, so, to begin with, we consider the simple join of a subspace r and a point x. The join exists only if $\mathrm{tr}(rx)\neq 1$; then we define

$$r\vee x=r+(1-r)x(1-r)/[1-\mathrm{tr}(rx)],$$

By using the identity $xrx=\mathrm{tr}(rx)x$, it is easy to verify that this is a projection and that it satisfies $x(r\vee x)=x$ and $x(r\vee x)=r$, as required. When x is a point x', this definition can be written

$$x'\vee x=2(x'-x)^2/\sigma^2_{x'x},\qquad \sigma^2_{x'x}=\mathrm{tr}(x'-x)^2$$

and the exceptional condition $\mathrm{tr}(x'x)=1$ is realized when $\sigma_{x'x}=0$, i.e., when the connection between the points is light-like. *Two points connected by a light signal have no join*, in the sense of the definition, because their separation is 0.

If r and s are two general subspaces, the join and meet of r and s are defined by

$$r\vee s=1-(1-r)(1-sr)^{-1}(1-s),$$
$$r\wedge s=1-(1-r)\vee(1-s)=r(r+s-sr)^{-1}s, \tag{3.4}$$

provided that the inverses $(1-sr)^{-1}$ and $(r+s-sr)^{-1}$ exist.

These formulas simplify considerably when r commutes with s; then, write $t=rs=sr$ so that $st=t=tr$ and it follows from $(1-s)=(1-s)(1-t)$, $(1-r)=(1-t)(1-r)$ and $(1-t)(1-t)^{-1}(1-t)=(1-t)$ that the join of r and s is $r\vee s=1-(1-s)(1-r)$, or $r\vee s=r+s-t$, whereas $r=r(r+s-sr)$ and $s=(r+s-sr)$, so that the meet of r and s is $r\wedge s=rs$. If $rs=sr$ but $t\neq 0$, then $r-t$ and $s-t$ are disjoint subspaces. If $t=0$, then $r\vee s=r+s$, $r\wedge s=0$ and the two subspaces are *disjoint*.

*More generally, even if r does not commute with s,

$$r\vee s=(1-s)r(1-sr)^{-1}+(1-r)s(1-rs)^{-1}=s\vee r,$$
$$r\wedge s=1-s(1-r)(r+s-sr)^{-1}-r(1-s)(r+s-rs)^{-1}=s\wedge r. \tag{3.5}$$

3.2 Classical Geometry of Space-Time

The four-dimensional space-time of the special theory of relativity, like the three-dimensional space of euclidean geometry, is flat, and is not, therefore, strictly compatible with the projective geometry introduced in the previous section. A flat (euclidean or pseudo-euclidean) geometry can be regarded either as a limiting example of a projective geometry, in which the curvature $1/R$ approaches zero, or as descriptive of a very small region in a projective geometry. Most contemporary models of the universe suggest that, at a particular time, space can be approximated by the three-dimensional spherical surface four dimensions, much as the surface of the earth can be approximated

by a two-dimensional sphere in three dimensions. In a spherical geometry, the straight lines and planes of Euclidean geometry are replaced by circles and spheres of radius R, which must be very large to provide a model of the observed universe; however, it is convenient for our purpose to adopt this radius R at some fixed time $x^0 = 0$ as the unit of length.

The simplest curved space-time is called de Sitter space, after its discoverer, in the context of the general theory of relativity. The matrix η in (3.3) has one negative eigenvalue, corresponding to the time-like dimension, and four positive eigenvalues, corresponding to the space-like dimensions and its elements η_{jk} are simply related to what is known as the metric tensor $g_{jk} = -\eta_{jk}$. Following the appearance in 1916 of Einstein's general theory of relativity, there has been a gradual acceptance of the idea that although three-dimensional physical space is curved and finite, a time coordinate could be chosen, that is *either* finite *or*, like the time in the special theory of relativity, could be extended arbitrarily far into the past. It became generally accepted, on the basis of the apparent recession of distant galaxies first noticed by Hubble, that the universe is expanding with time, and de Sitter's was the first model of the universe consistent with such observations. It does not include sufficient information to represent matter and gravity, but has the simple virtues admirably summarized in the aphorism of the Swiss Romansh: *Tuot ho sien temp e si'imsüra* (Everything has its time and everything has its limits)!

De Sitter's model differs from other simple models only in the choice of coordinates to represent distant events; his time coordinate may have arbitrarily large negative and positive values, so that the unobservable beginning of the universe, or 'big bang', if we choose to imagine that there was one, corresponds to time $x^0 = -\infty$, and the end of the universe, or 'big crunch', to time $x^0 = \infty$. In spite of the appearance of expansion, there is actually no beginning in time and no way of distinguishing one time from another. However, an important feature of de Sitter's model, and therefore of other models related to it by a change of coordinates, is that in a particular inertial frame, there is an horizon, or a set of points beyond which no light is transmitted to the observer; the observed energy and momentum of a photon from a distant source tends to zero near the horizon. Moreover, the horizon recedes as it is approached, so that if the distribution of sources of radiation of various types were uniform, the universe would have had much the same appearance to observers in the distant past. There are observations of 'background' microwave radiation, much of which has its origin in a concentration of sources near the horizon, and this at first seemed to be so uniform that it could only be attributed to a single event in the distant past. But an unambiguous interpretation of more recent data revealed fluctuations in the temperature of the background radiation much more consistent with emission from a multiplicity of sources. The ultimate interpretation of the data will depend on the accumulation of information derived from the actual observations, to identify

and correct for effects which do not depend on the geometrical model. Apart from their spatial distribution, the principal effects which need to be taken into account are:

(1) the change of apparent frequency, known as the Doppler effect, and the change in the apparent direction of the source, known as aberration, which both depend on the velocity, and so on the inertial frame, of the detector;

(2) a similar Doppler effect depending on the inertial frame of the source;

(3) the nature of the events forming the source, such as the ionic collisions which occur in a plasma, the ionization, recombination and orbital transitions in hydrogen and other atoms, and the annihilation of matter by anti-matter;

(4) the scattering and absorption of light by matter between the source and the detector; and

(5) the effect of variations in the gravitational field between the source and the detector.

The last is within the province of Einstein's theory of gravitation, but the other effects require the analysis of independent observations of a spectrum of radiation from distant sources, including the cosmic radiation which extends to the highest energies, and includes particles other than photons.

De Sitter's is undoubtedly the simplest model of the universe. In it, an event is represented in a projective four-dimensional space-time by a point, which may be identified with a real matrix x of degree 5, satisfying $x^2 = x$ and with elements which we shall denote by $-x^j x_k$, thus:

$$x = \begin{pmatrix} -x^0x_0 & -x^0x_1 & \dots & -x^0x_4 \\ x^1x_0 & x^1x_1 & \dots & x^1x_4 \\ \dots & \dots & \dots & \dots \\ x^4x_0 & x^4x_1 & \dots & x^4x_4 \end{pmatrix}, \qquad \sum_{j=0}^{4} x_j x^j = -1. \tag{3.6}$$

Clearly the element in the j-th row and k-th column is $x^j x_k$, with rows and columns numbered from 0 to 4. To conform with the usual notation we are choosing the contravariant and covariant vectors x^j and x_j so that their *space-like* components are opposite in sign ($x^j = -x_j$ for $j > 0$) but their time-like components x^0 and x_0 are equal. Then x is pseudo-symmetric, since the matrix η, defined so that $x_k = -\sum_{k=0}^{4} x^j \eta_{jk}$, has elements $\eta_{0j} = \eta_{j0} = -\delta_{0j}$ and $\eta_{jk} = \delta_{jk}$ for $j > 0$ and $k > 0$. Thus if the vectors x and $\bar{x}$ have components x^j and x_j respectively, we may rewrite (3.6) as

$$x = x\bar{x}, \qquad \mathrm{tr}(x) = \bar{x}x = 1 \qquad (\bar{x} = x\eta, \qquad \eta^{\mathrm{t}} = \eta, \qquad \eta^2 = 1), \tag{3.7}$$

where the product $x\bar{x}$ (in that order) is the matrix or outer product of the vectors x and $\bar{x}$, but $\bar{x}x$ (in that order) is the scalar or inner product. The projective condition $x^2 = x$ is automatically satisfied.

It is often useful to express the coordinates x^j in terms of the four pseudo-spherical coordinates (t, r, θ, φ), by writing

$$x^0 = \sinh t, \qquad x^1 = \sin r \cos\theta \cosh t, \qquad x^2 = \sin r \sin\theta \cos\varphi \cosh t,$$

$$x^3 = \sin r \sin\theta \sin\varphi \cosh t, \qquad x^4 = \cos r \cosh t, \tag{3.8}$$

where $r = \frac{1}{2}\pi$, in units of $R \simeq 10^{27}$ cm, corresponds to the most distant events on the horizon of the universe, and the time t is units of R/c, so that the velocity of light $\sin r / \sinh t$, in units of c, reduces to 1 near the origin at $r = t = 0$.

The apparent distance of the horizon for an observer at the origin increases with the time like $\cosh t$, but for events near the origin,

$$x^0 \simeq t, \qquad x^1 \simeq r\cos\theta, \qquad x^2 \simeq r\sin\theta\cos\varphi,$$

$$x^3 \simeq r\sin\theta\sin\varphi, \qquad x^4 \simeq 1 + \tfrac{1}{2}(t^2 - r^2),$$

so that x^0 can be identified with the time t, in the specified units, and (x^1, x^2, x^3) with the position vector of the event in cartesian coordinates. Thus in the local neighborhood of the origin, the components x^λ $(\lambda = 0, 1, 2, 3)$ may be identified with the coordinates x^λ of the special theory of relativity. The exact value of x^4 is $(1 + x_\lambda x^\lambda)^{\frac{1}{2}}$, involving only the invariant $x_\lambda x^\lambda$ (meaning $\sum_{\lambda=0}^{3} x_\lambda x^\lambda$) of the special theory of relativity. The separation $\sigma_{z'z}$ between events at the points z and z' is given by

$$\sigma_{z'z}^2 = \mathrm{tr}(x' - x)^2 = 2 - 2\sum_{j=0}^{4}(x'_j x^j)^2 \tag{3.9}$$

and the interval $\tau_{x'x}$, given by $\tau_{x'x}^2 = -\sigma_{x'x}^2$ reduces to $(x'_\lambda - x_\lambda)(x'^\lambda - x^\lambda)$, very nearly, in the neighborhood of the origin, as required by (3.1).

In classical physics, particles were idealized as points. The motion of a point in de Sitter space may be described by a matrix $x = x(\tau)$, and corresponding coordinates $x^j = x^j(\tau)$, depending on a single parameter τ, which can be chosen as the interval elapsed since the particle was at some initial point. The interval between two neighbouring points x and $x(\tau + d\tau) = x + dx$ is obtained by substituting $x' = x + dx$ and $x'_j = x_j + dx_j$ in (3.9), which then yields

$$d\tau^2 = -d\sigma^2 = -\mathrm{tr}(dx^2) = 2\sum_{j=0}^{4} dx_j x^j. \tag{3.10}$$

When $d\tau$ tends to zero, this expression is of second order, showing that the velocity vector $dx^j/d\tau$ of the particle is orthogonal to x^j, which should be expected since $\sum_{j=0}^{4} x_j x^j = -1$.

3.3 Changes of Observational Frame

We have now completed our introduction to the descriptive aspects of the geometry of physical space-time, in a matrix formulation. From the point of view of physics, the matrix formulation also provides a very convenient basis for the discussion of changes of the observational frame in a curved space. A change of this type is to be thought of as a change in the inertial frame of the physical system by means of which an observation is made; this may or may not be the same as that of a conscious observer. A particular inertial frame is used to specify an origin of spatial coordinates to which all other inertial frames are then related. The change of inertial frame may include a change of orientation, a change of velocity, a change of position in space and also a change of time. Although we shall be are here concerned with the representation of more complex information than is possible with a single qubit, we follow the terminology established in Chap. 2 and call a change of orientation a *rotation*, a change of velocity a *Lorentz transformation*, and a change of position or time a *translation*.

In a flat space a rotation and a translation in space are quite different concepts, but, as we have already seen in a more limited context in Sect. 2.5, a translation from one point to another in a curved space can be regarded as the result of a rotation about another very distant point which is unaffected by the rotation. Translations in space may therefore be classified as rotations. As a simple but familiar example, a translation along the equator on the two-dimensional surface of the earth is effected by a rotation about the north or south pole. In an $(n-1)$-dimensional space, there is an $(n-2)$-dimensional subspace, the centre of the rotation, consisting of points that are undisplaced by a rotation, and there is also a great circle, the *equatorial* circle, whose points are displaced but is undisplaced as a whole. The distance between any two points is unaffected by a translation in space or a rotation. A reflection also does not affect the distance between two points and could therefore be regarded as a kind of rotation, but it is one which usually requires movement out of physical space; for this reason, any movement that requires a reflection is classified as an *improper* rotation.

Since the inception of the special theory of relativity it has been accepted that the time between events depends on the velocity of the observational frame. As a consequence of this, just as, in our curved space-time, a translation in space is equivalent to a rotation, a translation in time is equivalent to a Lorentz transformation. *We may therefore consider Lorentz transformations at distant points as responsible for translational changes of the observational frame.*

As a result of any Lorentz transformation, the real matrices r, s, .. representing subspaces of the universe are changed to new real matrices r', s', ..., representing subspaces with the same dimensions: $\mathrm{tr}(r') = \mathrm{tr}(r)$, $\mathrm{tr}(s') = \mathrm{tr}(s)$, ... The transformation must not affect the separation of subspaces, as defined in (3.2), so that $\mathrm{tr}(r's') = \mathrm{tr}(rs)$, ... To satisfy these requirements, it is sufficient that each point x should be transformed to a corresponding point x', and we shall show that this can be achieved by similarity transformations similar to the rotations and boosts discussed in the

previous chapter. We write

$$x = \tfrac{1}{2}(1+w), \qquad x' = \tfrac{1}{2}(1+w'), \qquad xx'x = x\cos^2(\tfrac{1}{2}\chi) \tag{3.11}$$

where $\cos(\frac{1}{2}\chi) = \bar{x}'x$ if x and x' are factorized as in (3.7). Then χ is real when x and x' have space-like separation, but imaginary when they are separated by a time-like interval and $\bar{x}'x$ is greater than 1 in magnitude. In either event, $w^2 = w'^2 = 1$ and

$$ww' + w'w = 2\cos(\chi), \qquad (ww' - w'w)^2 = -4\sin^2(\chi),$$

so that, following a procedure similar to that leading to (2.36), we have

$$\begin{aligned} w' &= \tfrac{1}{2}(ww' + w'w + w'w - ww')w \\ &= \exp[\chi(w'w - ww')/\sin(\chi)]w \\ &= \exp[\tfrac{1}{4}\chi(w'w - ww')/\sin\chi]w\exp[-\tfrac{1}{4}\chi(w'w - ww')/\sin\chi] \end{aligned} \tag{3.12}$$

and

$$x' = u(x',x)xu^{-1}(x',x), \qquad u(x',x) = \exp[\tfrac{1}{4}\chi(w'w - ww')/\sin\chi]. \tag{3.13}$$

This is the required transformation, which is obviously very similar the transformations of qubits obtained in Sects. 2.3–2.5, but with the difference that, since x and x' are real, $w(x',x)$ is also real; for this reason, the transformation is said to be of orthogonal rather than hermitean type. But since in general the matrices $x\eta$ and $x'\eta$ are symmetric and x and x' are not, $(w'w - ww')\eta$ is antisymmetric though $w'w - ww'$ is not, the transformation is called *pseudo-orthogonal* rather than pseudo-hermitean.

In the theory of relativity a transformation may be regarded *either* as a relation between two points of space-time, *or* as a change in the inertial frame of the observer. Thus, if the point in space-time at which some event takes place is represented by the projective pseudo-symmetric matrix x in a particular inertial frame, we can take the view that the *same* point is represented by the matrix $x' = uxu^{-1}$, where u has the form shown in (3.13), in another inertial frame depending on u.

3.4 Events as Quantal Information

In quantum mechanics an event is associated with the emission or absorption of an elementary particle, normally a photon or other neutral particle, at some point of space-time. However, an event is, or should be, characterized by the quantal information to be obtained by detection of the emission or absorption of the particle. Apart from information concerning the existence of the particle, this information is what can be inferred from measurement of its energy and momentum. The momentum of an existing particle provides information concerning the direction of the source of the particle, and in a curved space-time the energy provides information concerning the distance of the particle from its source. Information to be derived from such a measurement is, therefore, geometrical in character and may be encoded in a pair of qubits, represented by a projective pseudo-hermitean matrix in a representation of degree 4. In general $2(m+1)$ qubits are required to represent a particular m-dimensional subspace of the universe, but for $m \leq 4$ this is possible in the same representation of the fourth degree. We shall begin by studying the structure of the matrices of degree 4, and in the next section shall show how they can be used to formulate a quantal geometry of space-time, practically equivalent to that constructed from the pseudo-symmetric matrices of degree 5, like x in Sect. 3.3, which represent points in the corresponding classical geometry.

If two qubits $n^{[1]}$ and $n^{[2]}$ are represented by matrices with elements $n^{[1]}_{j_1k_1}$ and $n^{[2]}_{j_2k_2}$ (where the subscripts take just two values, 1 and 2), the *direct product* of $n^{[1]}$ and $n^{[2]}$ is a matrix $n = n^{[1]} \otimes n^{[2]}$ of degree 4 with elements

$$n_{jk} = (n^{[1]} \otimes n^{[2]})_{jk} = n^{[1]}_{j_1k_1}n^{[2]}_{j_2k_2}. \tag{3.14}$$

In this instance the subscripts j and k could be defined by $j = 2(j_1-1)+j_2$ and $k = 2(k_1-1)+k_2$ which would then take values from 1 to 4, but there are some advantages in regarding them as *vectors* $j = (j_1, j_2)$ and $k = (k_1, k_2)$ which still take four different values when their components take the values 1 and 2. The matrix n defined in this way represents a segment of a 'tape' consisting of two qubits. Obviously the direct product $n^{[2]} \otimes n^{[1]}$ is different from $n^{[1]} \otimes n^{[2]}$ in general , just as the matrix product $n^{[2]}n^{[1]}$ is different from $n^{[1]}n^{[2]}$, but since it is a matrix of degree 4 it can be added to and multiplied by other matrices of the same degree, and multiplied by numbers in the usual way. It is therefore possible, and often convenient to express direct products as ordinary matrix products, and in this instance it is easily can be done by writing

$$n = n^{(1)}n^{(2)} = n^{[1]} \otimes n^{[2]}, \qquad n^{(1)} = n^{[1]} \otimes 1, \qquad n^{(2)} = 1 \otimes n^{[2]}, \tag{3.15}$$

where $n^{(1)}$ and $n^{(2)}$ are matrices with elements $n^{[1]}_{j_1k_1}\delta_{j_2k_2}$ and $\delta_{j_1k_1}n^{[2]}_{j_2k_2}$ respectively; although they are of degree 4, they represent qubits on the tape, and it is clear from (3.15) that $n^{(2)}n^{(1)}$ is not different from $n^{(1)}n^{(2)}$.

Like the qubit n in (2.17), the direct product of two qubits can be expressed as the tensor product of a spinor φ and a co-spinor $\bar{\varphi}$. Since $n^{[1]}_{j_1k_1} = \varphi^{[1]}_{j_1}\bar{\varphi}^{[1]}_{k_2}$ and $n^{[2]}_{j_2k_2} = \varphi^{[2]}_{j_2}\bar{\varphi}^{[2]}_{k_2}$, we have

$$n = \varphi\bar{\varphi}, \qquad n_{jk} = \varphi_j\bar{\varphi}_k, \qquad \varphi_j = \varphi^{[1]}_{j_1}\varphi^{[2]}_{j_2}, \qquad \bar{\varphi}_k = \bar{\varphi}^{[1]}_{k_1}\varphi^{[2]}_{k_2}, \tag{3.16}$$

where φ_j now has four components and may be called a *4-spinor*.

If the individual bits are subjected to independent transformations $n^{[1]} \to u^{[1]}n^{[1]}u^{[1]-1}$ and $n^{[2]} \to u^{[2]}n^{[2]}u^{[2]-1}$, where $u^{[1]}$ and $u^{[2]}$ are unitary, pseudo-unitary or real, according as $n^{[1]}$ and $n^{[2]}$ are hermitean, pseudo-hermitean or real, then n undergoes the transformation $n \to unu^{-1}$, where

$$u = u^{(1)}u^{(2)} = u^{[1]} \otimes u^{[2]}, \qquad u^{(1)} = u^{[1]} \otimes 1, \qquad u^{(2)} = 1 \otimes u^{[2]}.$$

3.4.1 Spin of the Photon

Particles of spin 1, such as the photon, provide a simple example. In the next chapter we shall consider particles of higher spin, including the photon, in a more general context, and we shall find that its spin is in a direction ξ normal to its polarization vector e, which is the direction of the oscillatory electric field of the photon, and is also normal to the direction of the associated magnetic field b:

$$\xi = e \times b = -\tfrac{1}{2}\mathrm{i}(eb - be), \qquad e = \sum_\alpha e_\alpha \sigma_a, \qquad b = \sum_\alpha b_\alpha \sigma_\alpha,$$

where $e^2 = b^2 = 1$ and $e \cdot b = 0$, so that the unit vectors ξ, e and b form an orthogonal triad. For spin 1 the state of a particle with spin in the direction $\boldsymbol{\xi}$ can be represented by a pair of similar qubits, thus:

$$n(\xi) = n^{(1)}(\xi)n^{(2)}(\xi) = n^{[1]}(\xi) \otimes n^{[2]}(\xi), \qquad n^{[1]}(\xi) = n^{[2]}(\xi) = \tfrac{1}{2}(1 + \xi).$$

The qubits $n^{(1)}(\xi)$ and $n^{(2)}(\xi)$ have factors depending on the electromagnetic field:

$$n^{[1]}(\xi) = n^{[2]}(\xi) = \tfrac{1}{2}(e + \mathrm{i}b)(e - \mathrm{i}b),$$

and satisfy $(e + \mathrm{i}b)n^{[1]}(\omega) = n^{[1]}(e - \mathrm{i}b) = 0$, as well as

$$\xi n^{[1]}(\xi) = n^{[1]}(\xi), \qquad \xi n^{[2]}(\xi) = n^{[2]}(\xi).$$

The matrix s representing the spin of the photon is given by

$$s = s^{(1)} + s^{(2)} = \sum_\alpha \xi_\alpha s_\alpha, \qquad s_\alpha = \tfrac{1}{2}(\sigma_\alpha^{(1)} + \sigma_\alpha^{(2)})\hbar$$

in terms of the Pauli matrices $\sigma_\alpha^{(1)}$ and $\sigma_\alpha^{(2)}$. Since $\sigma_\alpha^{(1)}$ and $\sigma_\beta^{(2)}$ commute, the components s_α of the spin satisfy $s_1 s_2 - s_2 s_1 = \mathrm{i}\hbar s_3$, etc. and the spin angular momentum vector of the photon is $\mathbf{s}$ in the representation space of the product of qubits. The generalization of this result for arbitrary spin will be found in the following chapter.

3.5 Fermions in Space-Time

In quantum mechanics the fundamental events are those resulting in the creation or annihilation of a particle, and these events form the sub-structure of space-time. As shown in Sect. 2.1, the creation and annihilation of a single fermion requires just one qubit for its representation, but the complete description of its state requires the combination of two qubits of different types, in the manner shown in (3.15). The types depend on whether the description is in terms of the coordinates or the momentum of the particle. We consider first the coordinate representation.

The simplest matrix representing a fermion in four-dimensional space-time is a direct product $n(\xi;\eta)$ of qubits $n(\xi)$ and $n(\eta)$ of hermitean and real types, which were considered in Sects. 2.3 and 2.5 respectively: Thus we have

$$n(\xi;\eta) = n(\xi)n(\eta), \qquad n(\xi) = \tfrac{1}{2}(1 + \xi), \qquad n(\eta) = \tfrac{1}{2}(1 + \eta),$$

$$\xi = \xi_1\sigma_1 + \xi_2\sigma_2 + \xi_3\sigma_3, \qquad \eta = \eta_1\tau_1 + \eta_2\tau_2 + \eta_0\tau_0, \tag{3.17}$$

where

$$\sigma_1^2 = \sigma_2^2 = 1, \qquad \tau_1^2 = \tau_2^2 = 1,$$

$$\sigma_1\sigma_2 = -\sigma_2\sigma_1 = \mathrm{i}\sigma_3, \qquad \tau_1\tau_2 = -\tau_2\tau_1 = \tau_0. \tag{3.18}$$

and though σ_2 is hermitean and imaginary, the matrices τ_1, τ_2, and τ_0 are all real.

In the previous chapter the qubits were given a geometrical interpretation. in which ξ was a unit vector in three dimensions, expressible in terms of polar angular variables (θ, φ), and η a unit vector in $2+1$ dimensions, expressible in terms of space-time variables (t, r), thus:

$$\xi_1 = \sin\theta\cos\varphi, \qquad \xi_2 = \sin\theta\sin\varphi, \qquad \xi_3 = \cos\theta,$$

$$\eta_1 = \cosh t \sin r, \qquad \eta_2 = \cosh t \cos r, \qquad \eta_0 = \sinh t. \tag{3.19}$$

Since $\xi^2 = \eta^2 = 1$, $n(\xi;\eta)$ may be factorized in various alternative ways, e.g.,

$$n(\xi;\eta) = \tfrac{1}{2}\, n(\xi)[1 + (\xi_1\sigma_1 + \xi_2\sigma_2 + \xi_3\sigma_3)\eta_1\tau_1 + \eta_2\tau_2 - \eta_0\tau_0)] = n(\xi)p(x)$$

where $p(x)$ is the pseudo-hermitean matrix

$$p(x) = \tfrac{1}{2}(1 + x), \qquad x = x^j\theta_j = x^0\theta_0 + x^1\theta_1 + x^2\theta_2 + x^3\theta_3 + x^4\theta_4, \tag{3.20}$$

and

$$x^0 = -\eta_0 \qquad x^1 = \xi_1\eta_1, \qquad x^2 = \xi_2\eta_1, \qquad x^3 = \xi_3\eta_1, \qquad x^4 = \eta_2,$$

$$\theta_0 = \tau_0, \qquad \theta_1 = \sigma_1\tau_1, \qquad \theta_2 = \sigma_2\tau_1, \qquad \theta_3 = \sigma_3\tau_1, \qquad \theta_4 = \tau_2. \tag{3.21}$$

Because $\xi^2 = \eta^2 = 1$, the matrix x also satisfies $x^2 = 1$. In geometrical terms, the matrix $p(x)$ is associated with a point in a four-dimensional projective space parametrized either by the coordinates (r, t, θ, φ) of (3.19), or by the coordinates x^j of the unit vector x in a five-dimensional pseudo-euclidean space. We shall therefore refer to x as a 5-vector.

Since $n(\xi;\eta)$ is a projective matrix, $p(x)$ in (3.20) is also projective and satisfies the idempotent condition $[p(x)]^2 = p(x)$.; but, although $\mathrm{tr}[n(\xi,\eta)] = 1$, $\mathrm{tr}[p(x)] = 2$.

The matrices θ_j of degree 4 in (3.21) are similar to Dirac matrices, whose properties and physical applications will be discussed more fully in the next section. However, they differ from the Dirac matrices in being associated with real qubits, rather than pseudo-hermitean qubits; they are therefore real and satisfy

$$\theta_j\theta_k + \theta_k\theta_j = 2\eta_{jk}, \qquad \eta_{jk} = -g_{jk} = \delta_{jk} - 2\delta_{j0}\delta_{k0}. \tag{3.22}$$

The coordinate x^4 is of special interest since it is the counterpart of the invariant η_2 of the real qubit which was considered in the last two sections of the previous chapter, and in string theory was found to be related to the invariant surface area of the string and hence to the action. The coordinate x^0 is identified with η_0 and is obviously a measure of the time. In de Sitter space an open string representing an isolated particle remains a two-dimensional surface, but now has a definite axis defining its position and direction of propagation, which with a suitably chosen origin and inertial frame may be chosen to coincide with the x^3-axis ($\theta = \varphi = 0$). If this is done, the coordinate x^3 is identified with η_1 and the results of Sect. 2.5 are unchanged. However, in de Sitter space strings with a variety of axes are possible, and may be simply related to one another by changes of the inertial frame. In the absence of interactions, a string terminates, or appears to do so, on a 'membrane' at the cosmological horizon. Current string theories suggest a dynamically determined radius for a string related to the Newtonian constant of gravitation and require the embedding of the string in a space of at least ten dimensions. Quantal embeddings of this type will receive detailed consideration later in Chap. 7.

There is no difficulty in generalizing the three-dimensional scalar and matrix vector products defined in (2.15) for five dimensions; thus, if x' is another 5-vector of the same type as x in (3.20),

$$x \cdot x' = \tfrac{1}{2}(xx' + x'x) = \eta_{jk}x^j x^{k\prime} = \cos\chi,$$

$$x \times x' = -\tfrac{1}{2}\mathrm{i}(xx' - x'x) = -\mathrm{i}\theta_{jk}x^j x^{k\prime} \tag{3.23}$$

where

$$\theta_{jk} = \tfrac{1}{2}(\theta_j\theta_k - \theta_k\theta_j). \tag{3.24}$$

But, like components of the spinor ψ in Sect. 2.5, the 'angle' χ may be imaginary when the product $x^0x^{0\prime}$ is sufficiently large. We note that, just as

for the vectors ξ and η in Sects. 2.3 and 2.4, the magnitudes of the vector and scalar products are related by

$$(x \times x')^2 = \tfrac{1}{2}(x' - x)\cdot(x' - x) = 1 - \cos^2\chi = \sin^2\chi \tag{3.25}$$

so that $(x \times x')/\sin\chi$ is always a unit vector, though $x \times x'$ may not be hermitean and $\sin^2\chi$ may then be negative.

As shown in Sects. 2.3 and 2.5, the qubits $n(\xi)$ and $n(\eta)$ can be transformed to other qubits $n(\xi')$ and $n(\eta')$ of the same type $n(\xi',\eta')$ by a rotation $u(\xi',\xi)$ and Lorentz transformation $v(\eta',\eta)$, respectively, thus:

$$n(x') = w(x',x)n(x)w^{-1}(x',x), \qquad w(x',x) = u(\xi',\xi)v(\eta',\eta). \tag{3.26}$$

However, the transformation matrix $w(x',x)$ can also be expressed as directly in terms of the vector product, thus:

$$w(x',x) = \exp[-\tfrac{1}{2}\mathrm{i}\chi(x\times x')/\sin\chi] = \cos(\tfrac{1}{2}\chi) - \mathrm{i}\sin(\tfrac{1}{2}\chi)(x\times x')/\sin\chi, \tag{3.27}$$

from which it follows that

$$w(x',x)xw^{-1}(x',x) = w^2(x',x)x = [\cos\chi - \mathrm{i}\sin\chi(x\times x')/\sin\chi]x$$

$$= \tfrac{1}{2}(xx' + x'x - xx' + x'x)x = x'.$$

To express $w(x',x)$ in terms of the θ-matrices, we note that, making use of (3.23), the result of (3.27) can be written

$$w(x',x) = \exp(-\tfrac{1}{2}\chi\theta_{jk}x^j x^{k\prime}/\sin\chi) \tag{3.28}$$

The θ_{jk} in (3.24) are therefore identified as generators, for spin $\frac{1}{2}$, of various types of transformations which form the de Sitter group $SO(4,1)$ in a space with four space-like and one time-like dimensions. Since $(\mathrm{i}\theta_{23}, \mathrm{i}\theta_{31}, \mathrm{i}\theta_{12}) = \frac{1}{2}(\sigma_1,\sigma_2,\sigma_3)$, these matrices are generators of a subgroup $SO(3)$ of rotations, and in units of $\hbar$ represent the components of the spin angular momentum $\mathbf{s}$ for a system of spin $\frac{1}{2}$, as described in Sect. 2.2. On the other hand, $(\theta_{01},\theta_{02},\theta_{12})$ are generators of a subgroup $SO(2,1)$ of rotations and Lorentz transformations, similar to that described in Sect. 2.4. In quantum mechanics, the set of matrices $(\theta_{01},\theta_{02},\theta_{03})$ is used to represent the *central vector* for a system of spin $\frac{1}{2}$. The central vector of any system is defined as the position vector of the centre of mass, multiplied by the mass, in units of $\hbar/c$; these units are so small that although different components of the central vector do not commute exactly, they do so very nearly.

In space-time, the entire Lorentz group $SO(3,1)$ includes rotations in three dimensions as well as Lorentz transformations, and therefore has all of the θ_{jk} as generators, except those with $j = 4$ or $k = 4$. In de Sitter space. The matrices $(\theta_{14},\theta_{24},\theta_{34})$ are generators of translations in space, or changes of position, in units of R, and θ_{04} is the generator of translations in

time, in units of R/c. In a cosmological context the matrices $(\theta_{14}, \theta_{24}, \theta_{34})$ may also be considered as generators of rotations and (in units of $\hbar$) act as components of the *orbital angular momentum* **l** of non-relativistic quantum mechanics. The approximations required in applications to non-relativistic and special relativistic quantum mechanics will be considered in more detail in Chap. 5.

The result of present importance is that the θ_{jk} are to be interpreted not only as generators of various types of transformations, but in the coordinate representation are the *fundamental quantal observables of a particle of spin half.*

3.5.1 Dirac's Equation

The γ-matrices first appeared in Dirac's special relativistic theory of the electron, but were subsequently used for corresponding theories of other particles of spin $\frac{1}{2}$, including the neutrino, though for a time it was thought that this was a massless particle with only left-handed spin. In what is known as the *interaction representation*, which in the coordinate representation is also correct for a particle *free of interactions*, Dirac's equation was usually written

$$\mathrm{i}\hbar\gamma^\lambda\partial_\lambda\psi(x) = mc\psi(x), \tag{3.29}$$

where $2\pi\hbar$ is Planck's constant, $\partial_\lambda = \partial/\partial x^\lambda$ $(\lambda = 0, 1, 2, 3)$, $\psi(x)$ is a 4-spinor of the type defined in (3.16), is the mass of the particle and c is the velocity of light. As usual, summation over all four values of the repeated greek affix λ is implied. The Dirac matrices γ^λ satisfy

$$\gamma^\lambda\gamma^\mu + \gamma^\mu\gamma^\lambda = 2g^{\lambda\mu}, \tag{3.30}$$

where $g^{00} = 1$ but $g^{\lambda\mu} = -\delta_{\lambda\mu}$ for $\lambda, \mu > 0$; they are analogues of the real θ^λ matrices introduced in (3.21), but are defined in terms of a pseudo-hermitean rather than a real qubit.

To take account of the interaction of an electron with an electromagnetic field with the scalar potential A^0 and vector potential $\mathbf{A} = (A^0, A^1, A^2)$, Dirac adopted the classical procedure of replacing the differential operator $\mathrm{i}\hbar\partial_\lambda$ representing the total energy–momentum of the particle energy with $\mathrm{i}\hbar\partial_\lambda - eA_\lambda$. Dirac's theory was soon recognized as giving a more accurate account than Schrödinger's equation of various phenomena, especially the fine structure of the energy spectrum of the hydrogen atom and the magnetic moment of the electron, and Dirac's equation subsequently became one of the fundamental equations in the very successful development of quantum electrodynamics and other field theories for the interaction of fermions and bosons. At the same time, it was recognized that it had limitations as a special relativistic equation and required generalization in the context of gravitation and cosmology, quite apart from the need to take account of weak and strong

interactions. In the following we shall give a generalization of Dirac's equation for curved space-time, leaving the further generalization for weak interactions and gravitation to be considered in Chap. 7.

At present we are concerned with the momentum representation, in which the covariant differential operator $\mathrm{i}\hbar\partial_\lambda$ of (3.29) is replaced by its eigenvalue k_λ, which in its contravariant form k^λ is the energy–momentum vector of a particle, or the negative of the energy–momentum of an antiparticle. We recall that in (2.38) and (2.39) the energy was defined by $E = \pm mc^2\omega_0$, and always greater than zero when the positive sign is chosen for a particle and the negative sign for an antiparticle. We shall retain this interpretation here, but are now able to identify all three components of the momentum as $\pm\mathbf{k}$. We shall also write $\kappa^j = k^j/mc$, so that κ^λ $(\lambda = 0, 1, 2, 3)$ is the velocity 4-vector of a particle, or the negative of the velocity 4-vector of an antiparticle.

The state of a free fermion is represented by the direct product $n(\xi;\omega)$ of the hermitean qubit $n(\xi)$ representing its spin and a time-like pseudo-hermitean qubit $n(\omega)$ representing its velocity. This is

$$n(\xi;\omega) = n(\xi)n(\omega), \qquad n(\xi) = \tfrac{1}{2}(1+\xi), \qquad n(\omega) = \tfrac{1}{2}(1+\omega),$$
$$\xi = \xi_1\sigma_1 + \xi_2\sigma_2 + \xi_3\sigma_3, \qquad \omega = \omega_0\rho_0 - \omega_1\rho_1 - \omega_2\rho_2. \tag{3.31}$$

Here we are using the ρ-matrices introduced in 2.5; to ensure that ω is a unit vector matrix, they must satisfy the same relations $\rho_0^2 = -\rho_1^2 = -\rho_2^2 = 1$ as in (2.12). Thus we may also write

$$n(\xi;\omega) = \tfrac{1}{2}n(\xi)[1 + \omega_0\rho_0 - \omega_1(\xi_1\sigma_1 + \xi_2\sigma_2 + \xi_3\sigma_3)\rho_1 - \omega_2\rho_2] = n(\xi)p(\kappa)$$

where $p(\kappa)$ is the projective matrix

$$p(\kappa) = \tfrac{1}{2}(1+\kappa), \qquad \kappa = \kappa^j\gamma_j \equiv \kappa^0\gamma_0 + \kappa^1\gamma_1 + \kappa^2\gamma_2 + \kappa^3\gamma_3 + \kappa^4\gamma_4,$$
$$\kappa^0 = \omega_0, \quad \kappa^1 = -\omega_1\xi_1, \quad \kappa^2 = -\omega_1\xi_2, \quad \kappa^3 = -\omega_1\xi_3, \quad \kappa^4 = -\omega_2,$$
$$\gamma_0 = \rho_0, \quad \gamma_1 = \sigma_1\rho_1, \quad \gamma_2 = \sigma_2\rho_1, \quad \gamma_3 = \sigma_3\rho_1, \quad \gamma_4 = \rho_2. \tag{3.32}$$

The Dirac matrices γ_j satisfy the relations

$$\gamma_j\gamma_k + \gamma_k\gamma_j = 2g_{jk}, \qquad g_{00} = 1, \qquad g_{jk} = -\delta_{jk} \qquad (j, k > 0). \tag{3.33}$$

The definitions of the γ_j in (3.32) have been chosen to agree with the notation most commonly used in the literature, where however the hermitean matrix $\mathrm{i}\gamma_4$ is often denoted by γ_5. Since $\sigma_1\sigma_2\sigma_3 = \mathrm{i}$ and $\rho_1\rho_2 = \mathrm{i}\rho_0$,

$$\gamma_4 = -\gamma_0\gamma_1\gamma_2\gamma_3 = \epsilon^{\lambda\mu\tau\rho}\gamma_\lambda\gamma_\mu\gamma_\tau\gamma_\tau/24, \tag{3.34}$$

where $\epsilon^{\lambda\mu\tau\tau} = -\epsilon_{\lambda\mu\nu\rho}$ is the contravariant form of the permutation symbol defined in (A.18), and the summation convention is applied to the repeated

greek affixes. This relation between the γ_j holds only in the two-bit representations of the Dirac matrices.

Like the θ-matrices, the Dirac matrices can be used to form the elements of a Lie algebra $so(4,1)$ of the de Sitter type. If

$$\gamma_{jk} = \tfrac{1}{2}[\gamma_j, \gamma_k], \tag{3.35}$$

it follows from (3.32) that $\mathrm{i}\gamma_{23}$, $\mathrm{i}\gamma_{31}$ and $\mathrm{i}\gamma_{12}$ are components of the vector $\boldsymbol{\sigma}$ which determines the spin angular momentum $\mathbf{s} = \frac{1}{2}\hbar\boldsymbol{\sigma}$; they are generators of rotations. Similarly, γ_{01}, γ_{02} and γ_{03} are generators of Lorentz transformations in the energy–momentum representation.

*The γ_{jk} satisfy the commutation relations

$$[\gamma_{jk}, \gamma_l] = g_{kl}\gamma_j - g_{jl}\gamma_k, \qquad [\gamma_{jk}, \gamma_{lm}] = g_{kl}\gamma_{jm} - g_{jl}\gamma_{km} - g_{km}\gamma_{jl} + g_{jm}\gamma_{kj}.$$

We have already interpreted $k^\lambda = mc\kappa^\lambda$ as the energy–momentum 4-vector of a particle. But the five-vector k^j includes an additional component k^4, which is a significant innovation. This fifth component k^4 increases as $mc\sin(r/R)$ with the distance r of the source of the particle from the observer in de Sitter space, so that the energy–momentum k^λ of particles transmitted from distant sources is attenuated by a factor $\cos(r/R)$ and is reduced to zero for sources on the cosmological horizon at $r = R$. It has no role in the special theory of relativity and is negligible for free particles created and annihilated in an inertial frame near $r = 0$ in the local neighborhood of the observer.

We note that the velocity 5-vector κ^j is a unit vector in an energy–momentum analogue of de Sitter space: if $\kappa_j = g_{jk}\kappa^k$, then $\kappa^j\kappa_j = 1$, so that

$$\kappa^2 = \tfrac{1}{2}\kappa^j\kappa^k(\gamma_j\gamma_k + \gamma_k\gamma_j) = g_{jk}\kappa^j\kappa^k = 1. \tag{3.36}$$

and κ is therefore a unit vector matrix. It follows that $p(\kappa)$ is an idempotent matrix satisfying $\kappa p(\kappa) = p(\kappa) = p(\kappa)\kappa$, and that $n(\kappa) = n(\xi, \omega)$ also satisfies

$$\kappa n(\kappa) = n(\kappa) = n(\kappa)\kappa. \tag{3.37}$$

Although not hermitean, $n(x)$ has real eigenvalues 0 and 1 and can be regarded as an observable representing a tape segment containing the essential information of a particle in the momentum representation.

According to (3.16), the direct product $n(\xi, \omega)$ can be expressed as the tensor product of 4-spinor $\varphi(\kappa) = \varphi(\xi, \omega)$ and a 4-cospinor $\bar{\varphi}(\kappa) = \bar{\varphi}(\xi, \omega)$, and it follows from (3.37) that $\kappa\varphi(\kappa) = \varphi(\kappa)$ and $\bar{\varphi}(\kappa)\kappa = \bar{\varphi}(\kappa)$. From (3.32) we have $\kappa = k^j\gamma_j/(mc)$, so that

$$k^j\gamma_j\varphi(\kappa) = mc\varphi(\kappa), \qquad \bar{\varphi}(\kappa)k^j\gamma_j = \bar{\varphi}(\kappa)mc. \tag{3.38}$$

In the context of the special theory of relativity, where $k^4 = 0$, these results enable us to construct solutions of Dirac's equation. If

$$\psi(x) = \varphi(\kappa)\exp(-\mathrm{i}k_\lambda x^\lambda), \qquad \bar{\psi}(x) = \bar{\varphi}(\kappa)\exp(\mathrm{i}k_\lambda x^\lambda), \tag{3.39}$$

we have $\mathrm{i}\partial_\lambda\psi(x) = k_\lambda\psi(x)$, and (3.27) reduces to the first of the equations (3.38). Thus (3.39) is a solution of (3.27) for particles if $k^0 > 0$ and for antiparticles if $k^0 < 0$.

*The equations

$$\mathrm{i}\hbar\gamma^\lambda\partial_\lambda\psi(x) = mc\psi(x), \qquad -\mathrm{i}\hbar\partial_\lambda\bar{\psi}(x)\gamma^\lambda = \bar{\psi}(x)mc, \tag{3.40}$$

satisfied by $\psi(x)$ and the corresponding cospinor $\bar{\psi}(x)$ are consistent, provided that $\bar{\psi}(x) = \psi^*(x)\gamma^0$, where $\psi^*(x)$ denotes the complex conjugate of $\psi(x)$.

From (3.32) it can be seen that κ is unchanged if the signs of the vector matrix ξ and the component ω_1 of $\boldsymbol{\omega}$ are both reversed. A second solution of Dirac's equation with the same energy–momentum is therefore obtained by these reversals. The two solutions can be distinguished by the eigenvalue ± 1 of the observable τ, given by

$$\tau = \boldsymbol{\sigma}\cdot\boldsymbol{\kappa}/\,|\,\boldsymbol{\kappa}\,|, \tag{3.42}$$

which determines whether the spin angular momentum $\frac{1}{2}\hbar\boldsymbol{\sigma}$ *is parallel or anti-parallel to its momentum* and is called the *helicity* of the particle. The helicity cannot be changed by a rotation of the coordinate axes; it can be reversed by a change from a right-handed to a left-handed system of axes, which changes the sign of ξ, but the definition of the helicity is made unambiguous by our requirement that the system of axes should be right-handed.

3.5.2 Charged and Neutral Particles

The solutions of Dirac's equation for the electron and other charged fermions are complex, and there is a relation between the γ^λ matrices and the θ^λ matrices of the coordinate representation. To obtain this relation, we introduce the four-dimensional matrix

$$\tilde{n} = \tfrac{1}{4}[1 + \mathrm{i}(\rho_0\tau_0 + \rho_1\tau_1 + \rho_2\tau_2)] \tag{3.43}$$

constructed from the τ's in (3.17) and the ρ's in (3.31); it follows from

$$(\rho_0\tau_0 + \rho_1\tau_1 + \rho_2\tau_2)^2 = -3 - 2\mathrm{i}(\rho_0\tau_0 + \rho_1\tau_1 + \rho_2\tau_2)$$

that $\tilde{n}^2 = \tilde{n}$ and since $\mathrm{tr}(\tilde{n}) = 1$, $\tilde{n}$ represents a qubit which can be included on a suitable 'tape'. Moreover, $\tau_\alpha\tilde{n} = \mathrm{i}\rho_\alpha\tilde{n}$, $(\alpha = 0, 1, 2)$, so that

$$\theta_j\tilde{n} = \mathrm{i}\gamma_j\tilde{n}. \tag{3.44}$$

A 'tape' containing the qubit $\tilde{n}$ therefore has a representation in which the relation $\theta^\lambda = \mathrm{i}\gamma^\lambda$ can be used to eliminate the imaginary unit from Dirac's equation (3.29). This relation is in fact appropriate for a charged particle, but

not for a neutral particle such as the neutrino, where the solution of Dirac's equation, like that of Maxwell's equations for the photon, is required to be real.

The reality of the spinor representing a neutrino can be secured by adopting, instead of Dirac's representation, what is known as the *Majorana representation* for the matrices γ^λ ($\lambda < 4$) and the spinor $\psi(x)$ in (3.39). The Majorana matrices $\tilde{\gamma}^\lambda$ and the Dirac matrices γ^λ and the corresponding 4-spinors $\psi_{\mathrm{M}}(x)$ and $\psi(x)$ are simply related by the special pseudo-unitary transformation

$$\tilde{\gamma}^\lambda = u_{\mathrm{M}}\gamma^\lambda u_{\mathrm{M}}^{-1}, \qquad \psi_{\mathrm{M}}(x) = u_{\mathrm{M}}\psi(x), \qquad u_{\mathrm{M}} = 2^{-\frac{1}{2}}(1+\gamma_2\gamma_4), \quad (3.45)$$

which leaves the imaginary Dirac matrices γ^0, γ^1 and γ^3 unchanged and makes $\tilde{\gamma}^2 = \gamma^4 = \rho_2$ also imaginary though $\tilde{\gamma}^4 = -\gamma^2 = -\sigma_2\rho_1$ is real. But as the $\mathrm{i}\tilde{\gamma}^\lambda$ are real, there are real solutions of the type

$$\psi_{\mathrm{M}}(x) = \psi_{\mathrm{e}}\cos(k_\lambda x^\lambda) + \psi_{\mathrm{o}}\sin(k_\lambda x^\lambda), \qquad \psi_{\mathrm{e}} = (\theta^\lambda k_\lambda/mc)\psi_{\mathrm{o}}$$

of the equations

$$\mathrm{i}\hbar\tilde{\gamma}^\lambda\partial_\lambda\psi_{\mathrm{M}}(x) = mc\psi_{\mathrm{M}}(x), \qquad -\mathrm{i}\hbar\partial_\lambda\bar{\psi}_{\mathrm{M}}(x)\tilde{\gamma}^\lambda = \bar{\psi}_{\mathrm{M}}(x)mc$$

in the Majorana representation.

There are also real solutions of Dirac's equation in terms of Dirac matrices, of the same form as (3.39), but they require the adoption of *a real representation $i = \pm\tau_0$ of the imaginary unit*, as shown in (A.16). This is possible only on a tape segment containing *three* qubits, of hermitean, pseudo-hermitean and real types. The generalization of the results of this section for particles of higher spin also requires tape segments containing more than two qubits, and will be considered in the following chapter.

3.6 Summary

The natural generalization of the qubit is the quantal 'tape', in Turing's terminology, consisting of an ordered sequence of qubits which may be of any of the three fundamental types described in Chap. 2. The applications considered in this chapter are mostly simple generalizations not requiring more than two qubits. They begin with an account of the extension to the space-time of the special theory of relativity of the projective geometry of Sect. 2.2 and the uses of this theory in developing cosmological models of the universe. Real qubits are made a basis for the representation of projective spaces of the type introduced by De Sitter for the universe, with the neglect of gravitational effects. This leads naturally to an account of the generalization of the theory of local Lorentz transformations, given in Sect. 2.4 which is followed by a formulation of a projective geometry applicable to space time

but capable of extension to projective spaces of a much more general type, and in Sect. 3.3 by an account of the various types of tranformations affecting the frame of reference of observations and the observer. Further applications are made to the description of events in terms of quantal information and finally to systems of fermions in terms of either their energy and momentum or of their space-time coordinates.

4. Quantal 'Tapes'

So far we have considered observables represented by a single quantal 'bit', or a pair of qubits. These could be of hermitean type, as in Sects. 2.1 and 2.2, or of pseudo-hermitean type, as in the last two sections. In quantal information processing, and in quantized field theory, the matrix representation of a 'tape', consisting of several or even many qubits of the same type, is required. This can be constructed by direct multiplication from the representations of the separate qubits, which may be but are not necessarily of the same type. The simplest example, where no more than two qubits were involved, was considered in Sect. 3.4.

We now consider 'tapes' consisting of any number, and even a countable infinity of qubits. The direct product of the matrices $n^{[1]}$, $n^{[2]}$, $n^{[3]}$, ... is

$$n = n^{[1]} \otimes n^{[2]} \otimes n^{[3]} ... = n^{(1)} n^{(2)} n^{(3)} ..., \tag{4.1}$$

where the matrix elements of n are explicitly

$$n_{jk} = (n^{[1]} \otimes n^{[2]} \otimes n^{[3]} ...)_{jk} = n^{[1]}_{j_1 k_1} n^{[2]}_{j_2 k_2} n^{[3]}_{j_3 k_3} ....$$

If there are N factors $n^{[r]}$ $(r = 1, 2, ...N)$ in the direct product, the matrix n is of the 2^N-th degree, and is finite if N is finite, but uncountably infinite if N is countably infinite, i.e., if the superscript a may take any integral value. The subscripts $j = (j_1, j_2, j_3 ...)$ and $k = (k_1, k_2, k_3 ...)$ are vectors with N components, each of which takes two values. The commuting factors $n^{(r)}$ of n in (4.1), called *segments* of the tape, are

$$n^{(1)} = n^{[1]} \otimes 1 \otimes 1 ..., \qquad n^{(2)} = 1 \otimes n^{[2]} \otimes 1 ..., \qquad n^{(3)} = 1 \otimes 1 \otimes n^{[3]} ... \tag{4.2}$$

and, like n, are matrices of the 2^N-th degree with trace $\mathrm{tr}(n^{(r)}) = 2^{N-1}$.

*The hermitean conjugate n^* of the segment n is the direct product $n^{[1]*} \otimes n^{[2]^*} \otimes n^{[3]*} ...$ of the hermitean conjugates of its bits, and n is hermitean if the bits are hermitean.

Since, as shown in (2.17), each of the qubits $n^{[r]}$ can be expressed as the tensor product of a simple spinor $\varphi^{[r]}$ and a corresponding cospinor $\bar{\varphi}^{[r]}$, the segment n can be expressed as the tensor product $\varphi\bar{\varphi}$ of a 2^N-dimensional spinor φ and a corresponding cospinor $\bar{\varphi}$, and has matrix elements given by

$$n_{jk} = \varphi_j \bar{\varphi}_k, \qquad \varphi_j = \varphi^{[1]}_{j_1} \varphi^{[2]}_{j_2} \varphi^{[3]}_{j_3} ..., \qquad \bar{\varphi}_k = \bar{\varphi}^{[1]}_{k_1} \bar{\varphi}^{[2]}_{k_2} \bar{\varphi}^{[3]}_{k_3} .... \tag{4.3}$$

A transformation of the direct product $n = n^{(1)}n^{(2)}n^{(3)}...$, such as $n \to unu^{-1}$, is effected with a unitary or pseudo-unitary matrix $u = u^{(1)}u^{(2)}u^{(3)}...$, where

$$u^{(1)} = u^{[1]} \otimes 1 \otimes 1..., \qquad u^{(2)} = 1 \otimes u^{[2]} \otimes 1..., \qquad u^{(3)} = 1 \otimes 1 \otimes u^{[3]}....$$

The matrices $u^{[1]}$, $u^{[2]}$, $u^{[3]}$, ... are not necessarily related, but some of the qubits forming a quantal tape are likely to be of the same type, and sectors of the tape consisting of such qubits may be subjected to transformations of a corresponding type.

There are two important applications which reduce large areas of physics to information theory, and will be noted immediately. Firstly, if the number of eigenvalues a_r of a quantal observable $a = \sum_r a_r g_r$ is finite or countable, then, like the $n^{(a)}$ in (4.2), *the projections g_r can be interpreted as segments of a quantal tape.* Secondly, if a set of 2^N disjoint points z, z', z'', z''' ... spans a projective space of $2^N - 1$ dimensions of the type considered in Chap. 3, *each point can be represented by a direct products of m qubits*:

$$z = n^{(1)}n^{(2)}..., \qquad z' = (1 - n^{(1)})n^{(2)}...,$$

$$z'' = n^{(1)}(1 - n^{(2)})..., \qquad z''' = (1 - n^{(1)})(1 - n^{(2)})....$$

For $N = 2$, the join of the points z and z' (a great circle) is $z + z' = n^{(2)}$; the join of z and z'' is $n^{(1)}$. In the course of this chapter we shall consider a variety of other important physical applications.

A second application allows the definition of an extended set of Dirac matrices γ_j $(j = 0, 1, ..6)$, satisfying the same relations

$$\gamma_j\gamma_k + \gamma_k\gamma_j = 2g_{jk}$$

as in (3.33):

$$\gamma_0 = \rho_0, \qquad \gamma_1 = \sigma_1\rho_1, \qquad \gamma_2 = \mathrm{i}\tau_0\sigma_2\rho_1, \qquad \gamma_3 = \sigma_3\rho_1,$$

$$\gamma_4 = \rho_2, \qquad \gamma_5 = \mathrm{i}\tau_1\sigma_2\rho_1, \qquad \gamma_6 = \mathrm{i}\tau_2\sigma_2\rho_1. \tag{4.4}$$

Since ρ_0, ρ_1, ρ_2 and σ_2 are imaginary, these matrices are all imaginary, and in that respect resemble the Majorana matrices $\tilde{\gamma}_\lambda$, but for $j < 5$ they coincide with the Dirac matrices when τ_0 is replaced by its eigenvalue $-\mathrm{i}$. The matrices of the extended set are connected by a relation

$$\gamma_6 = \mathrm{i}\gamma_0\gamma_1\gamma_2\gamma_3\gamma_4\gamma_5$$

similar to the relation (3.34) between the Dirac matrices. The hermitean conjugate of γ_j is $\gamma_j^\dagger = \gamma^j = g^{jk}\gamma_k$, with a diagonal metric tensor g_{jk} such that $g_{00} = g_{44} = g_{55} = 1$ but $g_{ab} = -\delta_{ab}$ $(a, b = 1, 2, 3)$, in agreement with (3.33) for affixes not greater than 4. This extended set of Dirac matrices has irreducible representations of degree $2^3 = 8$. They will be found useful in the theory of neutral particles such as the neutrino and photon, and also in the theory of gravitation to be presented in Chap. 7.

In some applications, like those considered in Sect. 4.1 below, a quantal tape has symmetries which makes some or even much of the information to be gained from the 'scanning' of the tape redundant. There is a matrix I_{ab} of 2^N-degree which interchanges the qubits $n^{[r]}$ and $n^{[b]}$ of n, leaving the others unchanged; this has elements given by

$$(I_{ab})_{jk} = \delta_{j_ak_b}\delta_{j_bk_a}\prod_{c\neq a,b}\delta_{j_ck_c}$$

The set of matrices $(I_{12}, I_{23}, ..)$ generate a group known as the *symmetric group* of permutations of the N qubits.The components $n^{(a)}$ and $n^{(b)}$ of n are interchanged by I_{ab}:

$$I_{ab}n^{(a)} = n^{(b)}I_{ab}, \qquad I_{ab}n^{(b)} = n^{(a)}I_{ab},$$

$$I_{ab}n^{(c)} = n^{(c)}I_{ab} \qquad (c \neq a, c \neq b).$$

If $n^{[r]} = n^{[b]}$, then $I_{ab}n = nI_{ab}$, and I_{ab} commutes with n. This applies in particular in the completely symmetric representations of particles with higher spin, to be considered in the next section, where all the factors of n are the same.

Further sections will be concerned with applications and in the representation of systems of similar particles, including photons and other bosons, where the individual qubits of information concern the existence of particles of a particular type.

4.1 Representation of States of Higher Spin

In Sect. 2.3 it was shown that the spin of a fermion or any other systems of spin $\frac{1}{2}$ could be represented by a single qubit. There is a simple generalization of this results for a particle of higher spin, such as a photon with spin 1, which carries essentially the same geometrical information. In this application, the qubits are all alike, and for an elementary particle of spin s, the information is encoded on a 'tape', represented by the direct product

$$n(\xi) = n^{[1]}(\xi) \otimes n^{[2]}(\xi) \otimes ...n^{[s]}(\xi) = n^{(1)}(\xi)n^{(2)}(\xi)...n^{(2s)}(\xi),$$

$$n^{(1)}(\xi) = n^{[1]}(\xi) \otimes 1 \otimes ..., \qquad n^{(2)}(\xi) = 1 \otimes n^{[2]}(\xi) \otimes ...,$$

$$n^{(s)}(\xi) = 1 \otimes 1 \otimes ...n^{[2s]}(\xi), \tag{4.5}$$

where

$$n^{[r]}(\xi) = \tfrac{1}{2}\left(1 + \xi^{(r)}\right) = \tfrac{1}{2}\left(1 + \xi_1\sigma_1^{[r]} + \xi_2\sigma_2^{[r]} + \xi_3\sigma_3^{[r]}\right)$$

and the $\sigma_\alpha^{[r]}$ $(r = 1, 2, ..2s;\ \alpha = 1, 2, 3)$ are Pauli matrices which for each value of r are identical with those appearing explicitly in (2.9).

As for spin $\frac{1}{2}$, we can define cartesian components s_α of the spin angular momentum of a particle with spin s as generators of rotations of the vector $\boldsymbol{\xi}$ about the coordinate axes. The uniform transformation changing $n(\xi)$ to $n(\xi')$ is effected with a rotation matrix $u(\xi', \xi)$ which is a direct product of unitary matrices $u^{[i]}(\xi', \xi)$ like those defined in (2.37):

$$n(\xi') = u(\xi', \xi)n(\xi)u^{-1}(\xi', \xi), \qquad u(\xi', \xi) = u^{[1]}(\xi', \xi) \otimes u^{[2]}(\xi', \xi) \otimes ...$$

In particular, if the rotation is through an angle χ about the ξ_α-axis, so that $\xi \cdot \xi' = \cos\chi$ and $\xi \times \xi' = \sigma_\alpha \sin\chi$, then $u^{[r]}(\xi', \xi) = \exp(-\frac{1}{2}\mathrm{i}\chi\sigma_\alpha^{[r]})$ and

$$u(\xi_\alpha, \xi) = \exp(-\tfrac{1}{2}\mathrm{i}\chi\sigma_\alpha^{[1]}) \otimes \exp(-\tfrac{1}{2}\mathrm{i}\chi\sigma_\alpha^{[2]}) \otimes ... \exp(-\tfrac{1}{2}\mathrm{i}\chi\sigma_\alpha^{[2s]}) = \exp(-\mathrm{i}\chi s_\alpha/\hbar),$$

$$s_\alpha = \tfrac{1}{2}\sum_{r=1}^{2s} \sigma_\alpha^{(r)}\hbar, \qquad \sigma_\alpha^{(1)} = \sigma_\alpha^{[1]} \otimes 1 \otimes ... \otimes 1, \qquad ... \qquad \sigma_\alpha^{(2s)} = 1 \otimes 1 \otimes ... \otimes \sigma_\alpha^{[2s]}. \tag{4.6}$$

Since the components of s_α do not commute, only one component can be measured experimentally by a particular detector. If the coordinates are chosen so that this component is in the ξ_3-direction, and as the eigenvalues of the $\sigma_3^{(r)}$ are -1 and 1, *the measured eigenvalue of $s_3/\hbar$ must be half-integral, with a minimum value of $-s$ and a maximum of s.* But, as

$$\sum_\alpha \xi_\alpha s_\alpha n(\xi) = (s\hbar)n(\xi),$$

$n(\xi)$ is an eigenmatrix corresponding to the eigenvalue $s\hbar$ of the component of the spin in the direction of the vector $\boldsymbol{\xi}$, and the state of a particle with spin in this direction is represented by $n(\xi)$.

It is easy to verify that, like the J_α in (2.31), the s_α satisfy the commutation relations of the Lie algebra $so(3)$:

$$s_\alpha s_\beta - s_\beta s_\alpha = \mathrm{i}h\sum_\gamma \epsilon_{\alpha\beta\gamma} s_\gamma, \tag{4.7}$$

where $\epsilon_{\alpha\beta\gamma}$ is the permutation symbol defined in (A.19), with values 1, -1 or 0 according as α, β and γ are an even permutation, an odd permutation, or not a permutation of the admissible subscripts 1, 2 and 3. Irrespective of the value of s, *these generators of rotations may therefore be identified as components of the spin angular momentum.* From (4.7) and $\sum_{\beta,\gamma} \epsilon_{\alpha\beta\gamma} s_\beta s\gamma = 0$ it follows that

$$s_\alpha \mathbf{s}^2 - \mathbf{s}^2 s_a = s_\alpha \sum_\beta s_\beta s_\beta - \sum_\beta s_\beta s_\beta s_\alpha$$

$$= \sum_\beta [(s_\alpha s_\beta - s_\beta s_\alpha)s_\beta + s_\beta(s_\alpha s_\beta - s_\beta s_\alpha)] = 0,$$

so that $\mathbf{s}^2$ is an invariant of the Lie algebra $so(3)$. As shown in Sect. A.6, in a representation with spin s, $\mathbf{s}^2$ has the eigenvalue $s(s+1)$.

4.1.1 'Tapes' for Particles of Higher Spin

In Sect. 3.5 we have discussed solutions of Dirac's equation for the 4-spinor $\psi(x)$, which was shown to be simply related to a factor $\varphi(\kappa)$ of the direct product of two qubits representing a particle of spin half in the momentum representation. In this section we shall obtain generalizations of this equation for free particles of higher spin, showing that they can be formulated in terms of matrix representations of segments of tapes consisting of qubits of the three fundamental types. The representations for charged particles will be considered first.

The fundamental observables of a *charged* elementary particle of spin s may be constructed from matrices representing qubits in a string of two segments of a quantal tape associated with spin and velocity respectively:

$$n(\xi; \omega) = n(\xi)n(\omega),$$

$$n(\xi) = n^{(1)}(\xi)n^{(2)}(\xi)...n^{(2s)}(\xi), \qquad n(\omega) = n^{(1)}(\omega)n^{(2)}(\omega)...n^{(2s)}(\omega) \tag{4.8}$$

The factor $n(\xi)$ is hermitean and $n(\omega)$ is pseudo-hermitean. The factors $n^{(q)}(\xi)$ and $n^{(q)}(\omega)$ of $n(\xi)$ and $n(\omega)$ and the unit vector matrices $\xi^{(q)}$ and $\omega^{(q)}$ on which they depend are given by

$$n^{(q)}(\xi) = \tfrac{1}{2}(1 + \xi^{(q)}), \qquad n^{(q)}(\omega) = \tfrac{1}{2}(1 + \omega^{(q)}),$$

$$\xi^{(q)} = \xi_1\sigma_1^{(q)} + \xi_2\sigma_2^{(q)} + \xi_3\sigma_3^{(q)}, \qquad \omega^{(q)} = \omega_0\rho_0^{(q)} - \omega_1\rho_1^{(q)} - \omega_2\rho_2^{(q)}),$$

where, for $q \neq r$, $\rho_\alpha^{(q)}$ and $\rho_\beta^{(r)}$ satisfy $\rho_\alpha^{(q)}\rho_\beta^{(r)} = \rho_\beta^{(r)}\rho_\alpha^{(q)}$ but for $q = r$ they satisfy the same relations as the ρ_α in (3.32), so that the $\omega^{(q)}$ are unit vector matrices. Thus, in the generalization of the construction of the projection matrix $p(\kappa)$ for spin $\frac{1}{2}$ in Sect. 3.5, we may also write

$$n(\xi; \omega) = n(\xi)p(\kappa), \qquad p(\kappa) = p^{(1)}(\kappa)p^{(2)}(\kappa)...p^{(s)}(\kappa)$$

where

$$p^{(q)}(\kappa) = \tfrac{1}{2}[1 + \omega_0\rho_0^{(q)} - \omega_1(\xi_1\sigma_1^{(q)} + \xi_2\sigma_2^{(q)} + \xi_3\sigma_3^{(q)})\rho_1^{(q)} - \omega_2\rho_2^{(q)}]$$

$$= \tfrac{1}{2}(1 + \kappa^{(q)}),$$

$$\kappa^{(q)} = \kappa^j\gamma_j^{(q)} \qquad (j = 0, 1, 2, 3, 4; \qquad q = 1, 2, ..2s). \tag{4.9}$$

As in (3.32), the components of the velocity 5-vector κ^j are

$$\kappa^0 = \omega_0, \qquad \kappa^1 = -\omega_1\xi_1, \qquad \kappa^2 = -\omega_1\xi_2, \qquad \kappa^3 = -\omega_1\xi_3, \qquad \kappa^4 = -\omega_2.$$

However, for *neutral* particles, we make use also of real qubits, so that we have

$$n(\xi;\omega,\eta) = n(\xi)n(\omega)n(\eta), \qquad n(\eta) = n^{(1)}(\eta)n^{(2)}(\eta)...n^{(2s)}(\eta),$$

$$n^{(q)}(\eta) = \tfrac{1}{2}(1+\eta^{(q)}), \qquad \eta^{(q)} = \eta = \eta_1\tau_1^{(q)} + \eta_2\tau_2^{(q)} - \eta_0\tau_0^{(q)},$$

instead of (4.8) and

$$n(\xi;\omega,\eta) = n(\xi)p(\kappa), \qquad p(\kappa) = p^{(1)}(\kappa)p^{(2)}(\kappa)...p^{(s)}(\kappa)$$

$$= \tfrac{1}{2}(1+\kappa^{(q)}), \qquad \kappa^{(q)} = \kappa^j\gamma_j^{(q)} \qquad (0 \le j \le 6; \qquad 1 \le q \le 2s).$$

instead of (4.9). The matrices $\gamma_j^{(q)}$ commute for different values of q, but for a particular value of q satisfy the same relations as the extended set of Dirac matrices in (3.33):

$$\gamma_j^{(q)}\gamma_k^{(r)} = \gamma_k^{(r)}\gamma_j^{(q)} \qquad (q \ne r), \qquad \gamma_j^{(q)}\gamma_k^{(r)} + \gamma_k^{(r)}\gamma_j^{(q)} = 2g_{jk} \qquad (q = r), \tag{4.10}$$

if g_{jk} is the metric tensor of the energy–momentum analogue de Sitter space, given by $g_{00} = 1$, $g_{jk} = -\delta_{jk}$ for $1 \le j,k \le 4$, and $g_{jk} = \delta_{jk}$ if $5 \le j,k \le 6$. These matrices can be constructed within a representation of a tape consisting of $6s$ qubits.

We assume that $\kappa^j\kappa_j = 1$, so that the $\kappa^{(q)}$ are always unit vector matrices, and $\kappa^{(q)}p(\kappa) = p(\kappa) = p(\kappa)\kappa^{(q)}$; moreover, if we write $n(\kappa) = n(\xi,\omega,\eta)$ we have also

$$\kappa^{(q)}n(\kappa) = n(\kappa) = n(\kappa)\kappa^{(q)} \qquad (q = 1,2,...2s).$$

According to (4.3), $n(\kappa)$ is the tensor product of a 2^N-dimensional spinor $\varphi(\kappa)$ and a corresponding cospinor $\bar\varphi(\kappa)$, which must satisfy

$$\kappa^j\gamma_j^{(q)}\varphi(\kappa) = \varphi(\kappa), \qquad \bar\varphi(\kappa)\kappa^j\gamma_j^{(q)} = \bar\varphi(\kappa).$$

Thus, if the velocity vector κ^j is expressed as $\kappa^j = k^j/m$ (in units with $c = 1$), where k^λ is the energy–momentum, we have

$$k^j\gamma_j^{(q)}\varphi(\kappa) = m\varphi(\kappa), \qquad \bar\varphi(\kappa)k^j\gamma_j^{(q)} = \bar\varphi(\kappa)m. \tag{4.11}$$

The square of an hermitean matrix is positive definite, and it follows from (4.10) that $\gamma_j^{(q)}$ is hermitean or anti-hermitan according as $g_{jk} = 1$ or $g_{jk} = -1$ for $k = j$. The hermitean conjugate of $\gamma_j^{(q)}$ is therefore $\gamma_j^{(q)\dagger} = \gamma^{(q)j} = g^{jk}\gamma_k^{(q)}$, and the cospinor $\bar\varphi(\kappa)$ is *not* the hermitean conjugate of the spinor $\varphi(x)$. However, since $\gamma^{(q)j} = \eta\gamma_j^{(q)}\eta$, where

$$\eta = \prod_{q=1}^{2s}(\mathrm{i}\gamma_0^{(q)}\tau_0^{(q)}), \tag{4.12}$$

we can define generalized conjugates

$$\bar\varphi = \varphi^\dagger\eta, \qquad \bar\gamma_j^{(q)} = \eta\gamma_j^{(q)\dagger}\eta = \gamma_j^{(q)} \tag{4.13}$$

in such a way that the second of the equations (4.11) is a consequence of the first. If, as for charged particles, $j \le 4$, the factors $\tau_0^{(q)}$ may be replaced by eigenvalues $-\mathrm{i}$ in (4.12).

In the context of the special theory of relativity, where $k^j = 0$ for $j > 3$, (4.11) can be converted to a set of equations similar to solutions of Dirac's equation. As in (3.39), we write

$$\psi(x) = \varphi(\kappa)\exp(-\mathrm{i}k_\lambda x^\lambda), \qquad \bar\psi(x) = \bar\varphi(\kappa)\exp(\mathrm{i}k_\lambda x^\lambda),$$

so that $\mathrm{i}\partial_\lambda\psi(x) = k_\lambda\psi(x)$, and (4.10) can be then rewritten as the set of differential equations

$$\mathrm{i}\hbar\gamma^{(q)\lambda}\partial_\lambda\psi(x) = m\psi(x), \qquad -\mathrm{i}\hbar\partial_\lambda\bar\psi(x)\gamma^{(q)\lambda} = \bar\psi(x)m. \tag{4.14}$$

Each of these equations has two solutions, distinguished by the eigenvalue $\tau = \pm 1$ of the helicity $\boldsymbol{\sigma}\cdot\boldsymbol{\kappa}/\,|\,\boldsymbol{\kappa}\,|$, where $\boldsymbol{\sigma} = 2\mathbf{s}/\hbar$ in terms of the spin angular momentum $\mathbf{s}$.

4.1.2 Matrices for Higher Spin

By summation over q, the equations (4.14) are reduced to

$$\mathrm{i}\hbar\alpha^\lambda\partial_\lambda\psi(x) = sm\psi(x), \qquad -\mathrm{i}\hbar\partial_\lambda\bar\psi(x)\alpha^\lambda = sm\bar\psi(x), \qquad \alpha_\lambda = \tfrac{1}{2}\sum_{q=1}^{2s}\gamma_\lambda^{(q)}, \tag{4.15}$$

which we shall regard as the generalization of Dirac's equation in the context of the special theory of relativity for charged particles of spin s. The factor $\frac{1}{2}$ has been included in the definition of the matrices α_λ to simplify their commutation relations; apart from that, it will be noticed that, since the $\gamma_\lambda^{(q)}$ are imaginary, the α_λ are also imaginary, and it is a consequence of (4.13) that the conjugate $\bar\alpha_\lambda = \eta\alpha_\lambda^\dagger\eta$ of α_λ is α_λ.

Before proceeding further, we shall discuss some important properties of the α-matrices, and, in doing so, for convenience shall consider the extended set α_j with $0 \le j \le 6$, expressed in terms of a set of matrices $\gamma_j^{(q)}$ in the same way as the α_λ to the $\gamma_\lambda^{(q)}$. We therefore write

$$\alpha_j = \tfrac{1}{2}\sum_{q=1}^{2s}\gamma_j^{(q)}, \qquad \alpha_{jk} = \tfrac{1}{4}\sum_{q=1}^{2s}(\gamma_j^{(q)}\gamma_k^{(q)} - \gamma_j^{(q)}\gamma_j^{(q)}), \tag{4.16}$$

in which the α_{jk} provide a generalization of the γ_{jk} defined in (3.35) for spin $\frac{1}{2}$. We note that

$$(\gamma_j^{(q)}\gamma_k^{(q)})\gamma_l^{(q)} - \gamma_l^{(q)}(\gamma_j^{(q)}\gamma_k^{(q)}) = 2\gamma_j^{(q)}g_{kl} - 2\gamma_k^{(q)}g_{jl}$$

is a consequence of (4.10), so that

$$\alpha_{jk}\alpha_l - \alpha_l\alpha_{jk} = g_{kl}\alpha_j - g_{jl}\alpha_k,$$

$$\alpha_{jk}\alpha_{lm} - \alpha_{lm}\alpha_{jk} = g_{kl}\alpha_{jm} - g_{jl}\alpha_{km} - g_{km}\alpha_{jl} + g_{jm}\alpha_{kl}. \qquad (4.17)$$

The second line shows that the α_{jk} satisfy the commutation relations of the Lie algebra $so(5,1)$, an extension of the de Sitter group; the first line shows that the α_{jk} and the α_l together satisfy the commutation relations of the extended algebra $so(5,2)$.

When $j \leq 4$, there are two-bit representations of the $\gamma_j^{(q)}$, and relations $\gamma_4^{(q)} = \epsilon^{\lambda\mu\nu\rho}\gamma_\lambda^{(q)}\gamma_\mu^{(q)}\gamma_\nu^{(q)}\gamma_\rho^{(q)}/24$ similar to (3.34), and, since $\epsilon^{\lambda\mu\nu\rho}(\gamma_\lambda^{(q)}\gamma_\mu^{(r)} + \gamma_\lambda^{(r)}\gamma_\mu^{(q)}) = 0$, when the α_λ are defined as in (4.16) there is a similar relation

$$\alpha_4 = \tfrac{1}{3}\,\epsilon^{\lambda\mu\nu\rho}\alpha_\lambda\alpha_\mu\alpha_\nu\alpha_\rho$$

for matrices of higher spin, which is usually assumed for charged particles. But for neutral particles the matrices are required to be real and *three-bit representations of the $\gamma_j^{(q)}$*, as defined in (4.10), *must therefore be used.* In these representations, the analogous relation between the α_j is

$$\alpha_6 = \tfrac{2}{45}\,\epsilon^{jklpqr}\alpha_j\alpha_k\alpha_l\alpha_p\alpha_q\alpha_r.$$

For values 1, 2 and 3 of the subscripts in (4.17), the α_{jk} are directly related to the cartesian components s_α of the spin angular momentum $\mathbf{s}$ defined in (4.6) by

$$(s_1, s_2, s_3) = \mathrm{i}\hbar(\alpha_{23}, \alpha_{31}, \alpha_{12}),$$

and the commutation relations are those of the Lie algebra $so(3)$ of the group of rotations, already given in (4.7). The spin s is the maximum eigenvalue of s_1, s_2 or s_3. On the other hand, if the subscripts are given the values 0, 1, 2 and 3, the $\alpha_{\lambda\mu}$ have the commutation relations of the Lie algebra $so(3,1)$ of the Lorentz group.

4.1.3 Spin 0 and 1

The simplest and most important application is to elementary particles of spin 1, which include the photon though this requires special consideration because of its vanishing mass. However, field equations for particles like the π-mesons of spin 0, which are not elementary, can also be formulated in terms of the *Kemmer matrices*

$$\beta_j = \tfrac{1}{2}\,(\gamma_j^{(1)} + \gamma_j^{(2)}) \qquad (s = 1). \qquad (4.18)$$

Apart from those which follow from the substitution of β_j for α_j in (4.16) and (4.17), they satisfy some relations which distinguish them from the Dirac matrices and other matrices for higher spin. To obtain these relations, we first use (4.10) to derive

$$\beta_j\beta_l + \beta_l\beta_j = g_{jl} + \tfrac{1}{2}\,(\gamma_j^{(1)}\gamma_l^{(2)} + \gamma_l^{(1)}\gamma_j^{(2)}),$$

and hence also

$$\beta_k(\beta_j\beta_l + \beta_l\beta_j) + (\beta_j\beta_l + \beta_l\beta_j)\beta_k = 2g_{jl}\beta_k + g_{jk}\beta_l + g_{kl}\beta_j.$$

Then, setting $\beta_{jk} = \beta_j\beta_k - \beta_k\beta_j$, we add the result

$$(\beta_{jk}\beta_l - \beta_l\beta_{jk}) + (\beta_{lk}\beta_j - \beta_j\beta_{lk}) = (g_{kl}\beta_j - g_{lj}\beta_k) + (g_{kj}\beta_l - g_{jl}\beta_k)$$

derived from (4.16) to obtain the desired fundamental relations

$$\beta_j\beta_k\beta_l + \beta_l\beta_k\beta_j = g_{jk}\beta_l + g_{kl}\beta_j. \qquad (4.19)$$

For values of the subscripts less than 5 the Kemmer matrices have irreducible representation of degree 1, 5 and 10. If the subscripts take values up to 6, with $\gamma_j^{(1)}$ and $\gamma_j^{(2)}$ defined as in (4.4), there are representations of degree 1, 7, 21, and 28. In the representations of degree 1, all matrices have a single element which is zero: $\beta_j = [0]$.

If ψ_q are the components of a vector in the representations of degree 5, the matrix elements of β_λ $(0 \leq \lambda \leq 3)$ may be defined by

$$(\beta_\lambda\psi)_q = g_{\lambda q}\psi_4 - g_{q4}\psi_\lambda \qquad (0 \leq q \leq 4). \qquad (4.20)$$

To confirm that these matrices satisfy (4.19), we notice that $g_{44} = -1$ and if $\rho < 4$,

$$(\beta_\lambda\psi)_\rho = g_{\lambda\rho}\psi_4, \qquad (\beta_\lambda\psi)_4 = \psi_\lambda,$$

$$(\beta_\lambda\beta_\mu\psi)_\rho = g_{\lambda\rho}\psi_\mu, \qquad (\beta_\lambda\beta_\mu\psi)_4 = g_{\mu\lambda}\psi_4,$$

$$(\beta_\lambda\beta_\mu\beta_\nu\psi)_\rho = g_{\lambda\rho}g_{\nu\mu}\psi_4, \qquad (\beta_\lambda\beta_\mu\beta_\nu\psi)_4 = g_{\mu\lambda}\psi_\nu,$$

so that (4.19) is verified for $0 \leq j, k, l \leq 3$. This representation is somewhat degenerate, since $\beta_4 = 0$, but is used for particles of spin 0.

In the representation of degree 7, the matrices β_j are imaginary but all components ψ_q of ψ are required to be real, so that (4.20) is replaced by

$$\mathrm{i}(\beta_j\psi)_q = g_{jq}\psi_6 - g_{q6}\psi_j \qquad (0 \leq j \leq 5, \qquad 0 \leq q \leq 6), \qquad (4.21)$$

and since $g_{66} = 1$, the introduction of the imaginary unit ensures that (4.19) is verified in a similar way for $0 \leq j, k, l \leq 5$.

The components of a corresponding vector ψ of the representations of degree 10 can be denoted by ψ_{qr} $(0 < q < r \leq 4)$, but it is convenient to

define also $\psi_{rq} = -\psi_{qr}$. The matrix β_λ in this representation can then be defined by

$$(\beta_\lambda\psi)_{qr} = g_{\lambda q}\psi_{r4} - g_{\lambda r}\psi_{q4} + g_{q4}\psi_{\lambda r} - g_{r4}\psi_{\lambda q}. \tag{4.22}$$

To confirm that the required relations are satisfied, we notice that, if ρ, σ and τ take values less than 4,

$$(\beta_\lambda\psi)_{\rho\sigma} = g_{\lambda\rho}\psi_{\sigma u} - g_{\lambda\sigma}\psi_{\rho u}, \qquad (\beta_{gl}\psi)_{\tau 4} = \psi_{\lambda\tau},$$
$$(\beta_\lambda\beta_\mu\psi)_{\rho\sigma} = g_{\lambda\rho}\psi_{\mu\sigma} - g_{\lambda\sigma}\psi_{\mu\rho}, \qquad (\beta_\lambda\beta_\mu\psi)_{\tau 4} = g_{\mu\lambda}\psi_{\tau 4} - g_{\mu\tau}\psi_{\lambda 4},$$
$$(\beta_\lambda\beta_\mu\beta_\nu\psi)_{\rho\sigma} = g_{\lambda\rho}(g_{\nu\mu}\psi_{\sigma 4} - g_{\nu\sigma}\psi_{\mu 4}) - g_{\lambda\sigma}(g_{\nu\mu}\psi_{\rho 4} - g_{\nu\rho}\psi_{\mu 4}),$$
$$(\beta_\lambda\beta_\mu\beta_\nu\psi)_{\tau 4} = g_{\mu\lambda}\psi_{\nu\tau} - g_{\mu\tau}\psi_{\nu\lambda},$$

so that (4.19) is verified also on this vector space.

There is also a *dual* representation of the β_j in which, if $\tilde{\psi}$ is any 10-vector, then $(\beta_j\tilde{\psi})_{rs} = \epsilon_{jrstu}\tilde{\psi}^{tu}$.

In the representation of degree 21, as $g_{66} = 1$, instead of (4.21) we define

$$\mathrm{i}(\beta_j\psi)_{qr} = g_{jq}\psi_{r6} - g_{jr}\psi_{q6} + g_{q6}\psi_{jr} - g_{r6}\psi_{jq}, \tag{4.23}$$

where $0 \le j \le 5$ and $0 \le q, r \le 6$, and (4.19) is again verified in a similar way.

From (4.15) with $s = 1$ and $j < 4$, it is clear that the Kemmer matrices of (4.18) have representations of degree 10 defined on a 4-spinor $\varphi(\kappa)$ for a particle of spin 1. The latter, and the corresponding spinor $\psi(x)$ in (4.14) satisfy the equations

$$\beta^j k_j\varphi(\kappa) = mc\varphi(\kappa), \qquad \mathrm{i}\beta^\lambda\partial_\lambda\psi(\kappa) = mc\psi(x), \tag{4.24}$$

where $k^\lambda k_\lambda = m^2c^2$. In terms of the components $\psi_{\rho\sigma}(x)$ and $\psi_{\tau 4}(x)$ of $\psi(x)$, the second of these equations can be written

$$\mathrm{i}(\partial_\rho\psi_{\sigma 4} - \partial_\sigma\psi_{\rho 4}) = mc\psi_{\rho\sigma}, \qquad \mathrm{i}\partial_\lambda\psi^\lambda_{\ \tau} = mc\psi_{\tau 4}. \tag{4.25}$$

These equations may be used for charged particles of spin 1 in a local inertial frame.

For neutral particles of spin 1 in a local inertial frame we adopt the representation in (4.23). There is a neutral elementary particle of spin 1, with a non-vanishing rest mass m, which plays a role in the weak interactions in the theory of electro-weak interactions. For a free photon, the rest-mass is zero, so that $k^\lambda k_\lambda = 0$ and, in special relativistic approximation, k^4 amd k^5 also vanish, but $k^j k_j = m^2c^2$ so that $k^6 = \pm mc$. We choose $k^6 = -mc$ and note that, according to (4.23), $(1 + \beta_6)\psi_{\tau 6} = 0$. Instead of (4.24) and (4.25), therefore we have

$$\mathrm{i}\beta^\lambda\partial_\lambda\psi(x) = mc(1 + \beta_6)\psi(x),$$
$$\partial_\rho\psi_{\sigma 5} - \partial_\sigma\psi_{\rho 5} = mc\psi_{\rho\sigma}, \qquad \partial_\lambda\psi^\lambda_{\ \tau} = 0, \tag{4.26}$$

respectively. In the following section, we shall see that, in the absence of charge, these equations are equivalent to Maxwell's equations.

4.2 Maxwell's Equations and the Photon

We begin our discussion of the required modification of (4.24) for the photon with a historical perspective. The quantum theory of radiation had its origins in Maxwell's formulation of the laws of the electromagnetic field as the differential equations

$$\nabla\cdot\mathbf{E} = 4\pi\epsilon, \qquad \nabla\times\mathbf{E} = -\partial_0\mathbf{B},$$
$$\nabla\cdot\mathbf{B} = 0, \qquad \nabla\times\mathbf{B} = \partial_0\mathbf{E} + 4\pi\mathbf{j}/c \tag{4.27}$$

connecting the electric intensity $\mathbf{E}$ and magnetic induction $\mathbf{B}$ of the field with its sources in the electric charge density ϵ and the electric current density $\mathbf{j}$, divided by the velocity of light c to render the equations in *Heavidside* units, which are simplest and in common use in quantum electrodynamics. In electrostatic units, ϵ and $\mathbf{j}$ are replaced ϵ_e and $\mathbf{j}_\mathrm{e}$, given $\epsilon = 4\pi\epsilon_\mathrm{e}$ and $\mathbf{j} = 4\pi\mathbf{j}_\mathrm{e}$, and in electromagnetic units the corresponding current density is $\mathbf{j}_\mathrm{m}$, where $\mathbf{j} = 4\pi c\mathbf{j}_\mathrm{m}$. In Gibbs' notation, the differential operators $\nabla\cdot$ and $\nabla\times$ represent the divergence and curl of the vectors that follow them. As usual, ∂_0 is the differential operator $\partial/\partial x^0$, where $x^0 = ct$ is proportional to the time t.

The first of Maxwell's equations, as listed in (4.27), is the differential form of Coulomb's law governing the electric field associated with a distribution of charge. The second is the formulation of Faraday's law of electromagnetic induction. The third is the magnetic equivalent of the first, but implies the absence of magnetic monopoles in nature. The fourth equation is based on Ampère's law, but the right side includes the 'displacement current' $\partial_0\mathbf{E}$, which Maxwell realized was necessary to ensure the conservation of electric charge. The third and the second of the equations, respectively, can be satisfied identically by setting

$$\mathbf{B} = \nabla\times\mathbf{A}, \qquad \mathbf{E} = -\nabla\varphi - \partial_0\mathbf{A}, \tag{4.28}$$

where φ and $\mathbf{A}$ are the *scalar and vector potentials* of the electromagnetic field.

The scalar invariant

$$L = \partial_0\varphi + \nabla\cdot\mathbf{A}$$

is undetermined by the equations, and can be given any value; in classical relativistic theories the *Lorenz gauge condition* $L = 0$ is often assumed, but it is also possible to take $L = \partial_0\varphi$, so that $\nabla\cdot\mathbf{A} = 0$, in what is known as the *Coulomb gauge*. When a gauge condition has been chosen, the first and fourth of the equations (4.27), together with some appropriate boundary conditions, allow the potentials and hence the electric and magnetic fields to be determined uniquely.

*Without fixing the gauge, the potentials satisfy the wave equations

$$\partial_0{}^2\varphi - \nabla^2\varphi = \epsilon + \partial L/\partial x^0, \qquad \partial_0{}^2\mathbf{A} - \nabla^2\mathbf{A} = \mathbf{j}/c - \nabla L.$$

Now in general the charge density ϵ and the current density $\mathbf{j}$ in Maxwell's equations can be regarded as the source of the electromagnetic field, but in a region free of such sources there may still be an electromagnetic field. But in such a region $\nabla \cdot \mathbf{E} = 0$, and, if first $\mathbf{B}$ and then $\mathbf{E}$ is eliminated from the equations, they yield

$$\partial_0{}^2\mathbf{E} - \nabla^2\mathbf{E} = 0, \qquad \partial_0{}^2\mathbf{B} - \nabla^2\mathbf{B} = 0. \tag{4.29}$$

Maxwell inferred that under such conditions, the electromagnetic field consisted of waves propagating with the velocity of light, and reached the remarkable conclusion that *light is a form of electromagnetic radiation.*

The general solution of the wave equations (4.29) can be obtained in any rectangular region R of unit volume by expansion in Fourier series, thus:

$$\mathbf{E} = \sum_k (\mathbf{e}_k e^{i\mathbf{k}\cdot\mathbf{x}} + \mathbf{e}_k^* e^{-i\mathbf{k}\cdot\mathbf{x}}), \qquad \mathbf{B} = \sum_k (\mathbf{b}_k e^{i\mathbf{k}\cdot\mathbf{x}} + \mathbf{b}_k^* e^{-i\mathbf{k}\cdot\mathbf{x}}), \tag{4.30}$$

and it follows from (4.28) that $\mathbf{k}\cdot\mathbf{e}_k = \mathbf{k}\cdot\mathbf{b}_k = 0$ and $\mathbf{b}_k = i\mathbf{k}\times\partial_0\mathbf{e}_k/\mathbf{k}^2$, so that the vectors $\mathbf{k}$, $\mathbf{e}_k$, and $\mathbf{b}_k$ are mutually orthogonal. On substitution from (4.30) into (4.29), the latter reduce to the ordinary differential equations

$$\partial_0{}^2\mathbf{e}_k + \mathbf{k}^2\mathbf{e}_k = 0, \qquad \partial_0{}^2\mathbf{b}_k + \mathbf{k}^2\mathbf{b}_k = 0, \tag{4.31}$$

as for harmonic oscillators of angular frequency k^0, where $k^0 = |\,\mathbf{k}\,|$.

It was another result of Maxwell's theory that the energy density $\mathcal{E}$ and momentum density $\mathcal{K}$ associated with the electromagnetic field are

$$\mathcal{E} = \tfrac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2), \qquad \mathcal{K} = \mathbf{E}\times\mathbf{B}/c \tag{4.32}$$

yielding a total energy and momentum of

$$\tfrac{1}{2}\int_R (\mathbf{E}^2 + \mathbf{B}^2)d^3x = \sum_k \mathbf{k}^2\mathbf{e}_k^*\cdot\mathbf{e}_k, \qquad \int_R \mathbf{E}\times\mathbf{B}d^3x/c = \sum_k k^0\mathbf{k}\mathbf{e}_k^*\cdot\mathbf{e}_k/c$$

within the rectangular region of unit volume considered.

The above results were consistent with Planck's discovery near the beginning of the twentieth century that the intensity of black-body radiation in the infra-red spectrum appeared to require 'quantization' in packets with energy $\hbar ck^0$ and momentum $\hbar\mathbf{k}$. But it was then only a matter of time before this discovery was interpreted as meaning that, in spite of its wave-like properties, electromagnetic radiation consists of quanta, or particles called photons. For a single photon with energy $c\hbar k^0$ and momentum $\hbar\mathbf{k}$, the Fourier coefficient $\mathbf{e}_k$ was not arbitrary but had to have a magnitude $(\hbar/k^0)^{\frac{1}{2}}$.

With the development of the special theory of relativity, it was found that Maxwell's equations could be expressed concisely in terms of a *four-vector potential* A^λ with the time-like contravariant component φ, and the

electromagnetic field tensor $F_{\lambda\mu}$ with components identified with those of $\mathbf{E}$ and $\mathbf{B}$:

$$F_{\lambda\mu} = \partial_\lambda A_\mu - \partial_\mu A_\lambda, \qquad A_\mu = \eta_{\mu\nu}A^\nu,$$
$$A^0 = \varphi, \qquad (F_{23}, F_{31}, F_{12}) = \mathbf{B}, \qquad (F_{10}, F_{20}, F_{30}) = \mathbf{E}. \tag{4.33}$$

The first of these equations is equivalent to (4.28) and in this notation the first and last of equations (4.27) become

$$\partial_\mu F^{\lambda\mu} = j^\lambda/c, \tag{4.34}$$

where $j^0 = c\epsilon$. Since $F^{\lambda\mu}$ is anti-symmetric, we obtain, as an immediate consequence of this equation, $\partial_\lambda j^\lambda = 0$, which implies the conservation of electric charge.

In empty space, and also in the application to a single photon which has no interactions with charge or current, the right side of (4.34) may be omitted. Then, if

$$\psi_{\rho\sigma} = F_{\rho\sigma}, \qquad \psi_{\tau 6} = mcA_\tau, \tag{4.35}$$

the first of the equations (4.33) and (4.35) are equivalent to (4.26). We may therefore regard (4.34) as the wave equation for the photon.

4.3 Systems of Fermions

In this section we shall obtain representation of a system of fermions, such as electrons, of the same type. For such particles, according to Pauli's *exclusion principle, it is not possible for more than one fermion of a particular type to exist in the same state at the same time.* The state is specified by the eigenvalues of a set of commuting observables, such as the energy, momentum and spin direction, or, as for an electron in an atom, the energy, the orbital angular momentum and the spin angular momentum. The exclusion principle has an important application to the periodic table of the atomic elements; without it, for example, there would be nothing to prevent all three electrons in a lithium atom from occupying a state with zero orbital angular momentum. In quantized field theory, a fermion is usually supposed to be created and annihilated in a state with particular eigenvalues $(s, \mathbf{k})$ of the spin and the momentum, which determines the energy.

Since the number of possible momenta is infinite, the representation required for a complete set of creation and annihilation operators is uncountably infinite. However, in a finite volume, even of the size of the universe, the momenta have discrete values, and not only is the number of momentum states countably infinite but the number of qubits actually occupying these states at any time may be assumed to be finite. Though the 'tape' representing the states is therefore infinite in length, it is countably so, and the qubits with non-zero eigenvalues occupy only a finite part of the tape. If the number

of qubits with eigenvalue 1 in a particular state S is m_S, this is an eigenvalue of an observable m, and the tape is represented by a minimal projection n (with trace $\mathrm{tr}(n) = 1$), such that

$$m = n^{(1)} + n^{(2)} + n^{(3)} + ..., \qquad n = n^{(1)}n^{(2)}n^{(3)}.... \tag{4.36}$$

As shown in (4.2), the elementary constituents $n^{(r)}$ are expressible in terms of qubits $n^{[r]}$ of the type already considered in Sect. 2.1, where it was shown that any qubit $n^{[r]}$ or its complement $1 - n^{[r]}$ could be expressed as the outer product of a pair of vectors. For any particular value of r the corresponding constituent $n^{(r)}$ of the tape can therefore also be resolved into factors, thus: $n^{(r)} = \psi^{(r)}\bar{\psi}^{(r)}$, with the inner product $\bar{\psi}^{(r)}\psi^{(r)} = 1$; similarly and $1 - n^{(r)} = \psi_c^{(r)}\bar{\psi}_c^{(r)}$ where $\bar{\psi}_c^{(r)}\psi_c^{(r)} = 1$ and $\bar{\psi}^{(r)}\psi_c^{(r)} = \bar{\psi}_c^{(r)}\psi^{(r)} = 0$. Since $n^{(r)}$ is hermitean, $\bar{\psi}^{(r)}$ and $\bar{\psi}_c^{(r)}$ can be chosen as complex conjugates of $\psi^{(r)}$ and $\psi_c^{(r)}$, respectively. Matrices corresponding to $\bar{f}$ and f in Sect. 2.1 are then defined as the outer products $\bar{f}_r = \psi^{(r)}\bar{\psi}_c^{(r)}$ and $f_r = \psi_c^{(r)}\bar{\psi}^{(r)}$, so that $n^{(r)} = \bar{f}_r f_r$ and $f_r n^{(r)} = (1 - n^{(r)})f_r$. In the present context, $n^{(r)}$ is only one of a countably infinite set $(n^{(1)}, n^{(2)}, n^{(3)}, ...)$ of constituents of a tape and, for all values of r, the relations

$$n^{(r)} = \bar{f}_r f_r = 1 - f_r\bar{f}_r, \qquad f_r^2 = \bar{f}_r^2 = 0. \tag{4.37}$$

are satisfied.

However, defined in this way, $\bar{f}_r$ and f_r commute with $\bar{f}_s$and f_s for $r \neq s$ and therefore do not conform with all the criteria required of fermion creation and annihilation matrices. To satisfy the exclusion principle it is necessary that when r and s are different these matrices should *anti-commute* and we therefore define these by $\bar{e}_1 = \bar{f}_1$ and $e_1 = f_1$, and

$$\bar{e}_r = (\prod_{s=1}^{r-1}\xi^{(s)})\bar{f}_r, \qquad e_r = (\prod_{s=1}^{r-1}\xi^{(s)})f_r \tag{4.38}$$

for $r > 1$, where

$$\xi^{(1)} = \xi^{[1]} \otimes 1 \otimes 1..., \qquad \xi^{(2)} = 1 \otimes \xi^{[2]} \otimes 1..., \qquad ....$$

and $\xi^{[r]}$ is the analogue of ξ in Sect. 2.1, given by $n^{[r]} = \frac{1}{2}(1 + \xi^{[r]})$. Then since $\xi^{(r)}f_r = -f_r\xi^{(r)}$ and $\xi^{(r)}\bar{f}_r = -\bar{f}_r\xi^{(r)}$, the *anti-commutators* of the creation and annihilation operators are

$$\{f_r, \bar{f}_s\} \equiv f_r\bar{f}_s + \bar{f}_s f_r = \delta_{rs}, \qquad \{f_r, f_s\} \equiv f_r f_s + f_s f_r = 0,$$

$$\{\bar{f}_r, \bar{f}_s\} \equiv \bar{f}_r\bar{f}_s + \bar{f}_s\bar{f}_r = 0. \tag{4.39}$$

for all values of r and s.

The above anti-commutation relations are characteristic of particles satisfying *Fermi–Dirac* statistics. Since, in particular, $(\bar{e}_r)^2 = 0$, it is not possible to create a state with two or more particles of the same type in the same state, e.g., with the same spin and momentum. In Sect. 6.1, creation and annihilation operators satisfying the above anti-commutation relations will be used to construct quantized field variables for electrons and other particles of spin $\frac{1}{2}$.

4.4 Bosons

The earliest known form of quantum statistics was discovered in principle in 1924 by S.N. Bose, and following an important contribution by Einstein became known as *Bose–Einstein* statistics. The most fundamental boson from the point of view of information theory is the photon, but bosons include other particles or systems of particles, such as mesons, and atomic nuclei like He^4 with integral spin. Their common feature is that there is no restriction on the number of bosons of a particular type that may exist in the same state, which is usually characterized by the eigenvalues of the spin and the momentum. This has important consequences and applications in the theory of observation, in laser physics, in quantized field theory, and in the phenomena of superfluidity and superconductivity.

Information concerning the physical environment reaches the observer through all the senses, but of these the most significant for many purposes is sight, or sensitivity to light. The transmission of light is not only the primary source of our perception of the geometrical relations between events and the variety of colour in the immediate environment and in the more distant universe, but forms the basis for the recording, transmission and retrieval of information in all visually accessible forms. Optical processing has advantages over electronic processing that are likely to make it the preferred method of information processing in the future. At the microscopic level, the carriers of optical information are photons, and the capacity of a single photon to stimulate the emission of other photons with the same spin and momentum has found important applications in the development of laser technology. A laser beam is a good approximation to a quantal tape, and potentially the carrier of an unlimited amount of information.

In quantized field theory it is possible for any number of identical bosons to be created in the same state, and this number may not therefore be represented as a single qubit. In fact, the complete set of states of bosons with the same spin and momentum must be represented by a quantal 'tape' of infinite length, and in the course of this section we shall examine the structure of the information, expressed in qubits, on a tape of this kind.

The more complex phenomena of superfluidity and superconductivity can also be subjected to analysis in the light of information theory, but an adequate discussion lies beyond the scope of this book.

We have already seen that, even before the discovery of quantum mechanics it was inferred from these results that the electromagnetic field in a region of finite volume was dynamically equivalent to a countably infinite set of harmonic oscillators. In the quantum theory of the electromagnetic field which was developed in 1925 by Born, Heisenberg and Jordan these results were formally unchanged, but the Fourier coefficients $\mathbf{e}_k$ and $\mathbf{b}_k$ were replaced with matrices, and it was shown that they were *quantized in amplitude*, in a way consistent with the presence of only integral numbers of photons in a state with a given momentum $\mathbf{k}$ and spin s within the region considered. This, together with Bose's earlier discovery of quantum statistics, led directly to the subsequent successes of quantum electrodynamics. In the following, we shall shall treat the number N of photons with a particular momentum and spin as an observable and express this matrix in terms of the elements of a quantal tape. The same considerations apply to any particles of integral spin and are therefore not restricted in their application to light. In many applications creation and annihilation matrices are needed for bosons as well as fermions, and the structure of these matrices will be our primary interest.

4.4.1 The Factorization Technique

We first give a concise account of the application of the more traditional approach, based on a factorization of the infinite matrix representing the complete tape for bosons of a particular type. As already foreshadowed, the number of bosons in a particular state, usually distinguished by their spin and momentum, will be denoted by N; this is not itself a projection but an observable with arbitrary non-negative integral eigenvalues N_j.

The creation and annihilation operators which change the eigenvalue of the matrix N appear naturally in the factorization method used to determine the eigenvalues of observables of that type in Sect. A.4, where the factors are denoted by $\bar{c}$ and c. Here the eigenvalues $(0, 1, 2, ...)$ are already known, and since the least eigenvalue is 0, the matrix N, like $n^{(r)}$ in (4.37), may be factorized in the form $N = \bar{b}b$. The theory of Sect. A.4 also shows that the eigenvalues of the matrix $N' = b\bar{b}$ are then $1, 2, 3, ...$, so that

$$b\bar{b} = N + 1, \qquad b\bar{b} - \bar{b}b = 1. \tag{4.40}$$

The simplest representation for these matrices is the one in which N is diagonal, with ascending eigenvalues along the principal diagonal; then c and $\bar{c}$ are codiagonal:

$$N = \begin{matrix} 0&0&0&0&\dots \\ 0&1&0&0&\dots \\ 0&0&2&0&\dots \\ 0&0&0&3&\dots \\ \dots&\dots&\dots&\dots&\dots \end{matrix}, \quad \bar{b} = \begin{matrix} 0&0&0&0&\dots \\ 1&0&0&0&\dots \\ 0&\sqrt{2}&0&0&\dots \\ 0&0&\sqrt{3}&0&\dots \\ \dots&\dots&\dots&\dots&\dots \end{matrix}, \quad b = \begin{matrix} 0&1&0&0&\dots \\ 0&0&\sqrt{2}&0&\dots \\ 0&0&0&\sqrt{3}&\dots \\ 0&0&0&0&\dots \\ \dots&\dots&\dots&\dots&\dots \end{matrix}.$$

It is a consequence of (4.29) that

$$N\bar{b} = \bar{b}(N + 1), \qquad Nb = b(N - 1), \tag{4.41}$$

and hence that $\bar{b}$ and b *may be interpreted as creation and annihilation matrices for bosons in the* chosen *state.* It will be noticed that these relations satisfied by b and $\bar{b}$ are similar to the corresponding relations satisfied by the fermion matrices f_r and $\bar{f}_r$ in (4.37), apart from the sign of $1 - f_r\bar{f}_r$. However, the difference of sign has the consequence that, if ν is any positive integer, $\bar{b}^\nu$ and b^ν do not vanish, and indeed it follows from (4.40) and (4.41) that

$$\bar{b}^\nu b^\nu = \bar{b}^{\nu-1}(N + 1)b^{\nu-1} = \bar{b}^{\nu-1}b^{\nu-1}(N + \nu) = (N + 1)...(N + \nu)$$

and similarly that $b^\nu\bar{b}^\nu = N...(N - \nu + 1)$. The eigenvalues of $\bar{b}^\nu b^\nu$ and $b^\nu\bar{b}^\nu$ in the vacuum are ν and 0 respectively.

4.4.2 The Tape Constructed from Qubits

In this application of information theory, we make use of the fact that the non-negative integral eigenvalues of the observable N are binary integers, or sequences of classical bits, which can be treated as eigenvalues of corresponding qubits. This approach has an important advantage in many applications where only the first qubit, or the first few qubits of the string have non-zero eigenvalues, so that the theoretically infinite length of the tape can be disregarded. The observable is

$$N = \sum_{j=1}^{\infty} 2^{j-1} n^{(j)}, \tag{4.42}$$

where each $n^{(j)}$ $(j = 1, 2, 3, ...)$ is a projection, with only two eigenvalues $n_0^{(j)} = 0$ and $n_1^{(j)} = 1$, and is therefore an element of a tape like that shown in (4.2), corresponding to a qubit $n^{[j]}$. In a measurement of N, the eigenvalue $n_k^{(j)}$ $(k = 0$ or $1)$ of $n^{(i)}$ is the j-th binary digit of the measured value $N_k = \sum_j 2^{j-1} n_k^{(j)}$. Since the eigenvalue N_k is finite, the summation over j always extends only up to some finite value. The elements $n^{(j)}$ can be resolved into factors $\bar{c}_j$ and c_j in the same way as for fermions, shown in (4.37):

$$n^{(i)} = \bar{c}_j c_j = 1 - c_j\bar{c}_j, \qquad \bar{c}_j^2 = c_j^2 = 0. \tag{4.43}$$

Now the boson creation and annihilation matrices $\bar{b}$ and b satisfying the relations (4.40) and (4.30) will be expressed in terms of the $\bar{c}_j$ and c_j. The former have the effect of increasing or decreasing any eigenvalue N_l of N by one unit, and this always changes the eigenvalue $n_l^{(1)}$ of $n^{(1)}$ to $1 - n_l^{(1)}$. But in the creation of a boson, if the eigenvalues $n_l^{(j)}$ are 1 for $j = 1, ...k$, they are

changed to 0, and $n_l^{(k+1)}$ is changed to 1 if it is 0; then $\bar{b}$ is a linear combination of the matrices $\bar{c}_1$, $c_1\bar{c}_2$, ... $c_1c_2...c_k\bar{c}_{k+1}$. Similarly, in the annihilation of a boson, if the first k of the eigenvalues $n_l^{(j)}$ are 0, they are changed to 1 and $n_l^{(k+1)}$ is changed to 0 if it is 1, so that b is a linear combination of the matrices c_1, $c_2\bar{c}_1$, ... $c_{k+1}...\bar{c}_2\bar{c}_1$. We may therefore write

$$\bar{b} = \lambda_1^{\frac{1}{2}}\bar{c}_1 + \lambda_2^{\frac{1}{2}}c_1\bar{c}_2 + \lambda_3^{\frac{1}{2}}c_1c_2\bar{c}_3 + ...,$$

$$b = \lambda_1^{\frac{1}{2}}c_1 + \lambda_2^{\frac{1}{2}}c_2\bar{c}_1 + \lambda_3^{\frac{1}{2}}c_3\bar{c}_2\bar{c}_1 + ..., \qquad (4.44)$$

where the coefficients $\lambda_k^{\frac{1}{2}}$ will necessarily depend on all the $n^{(j)}$ with $j > k$, *but not on those with* $j \leq k$.

The λ_k in (4.44) must now be chosen to satisfy the required relation $N = \bar{b}b$. This choice is made by using the condition that the expansion of N obtained from (4.3) with (4.43) and

$$\bar{b}b = \lambda_1 n^{(1)} + \lambda_2 n^{(2)}(1 - n^{(1)}) + \lambda_3 n^{(3)}(1 - n^{(2)})(1 - n^{(1)}) + ... \qquad (4.45)$$

should be the same. Without affecting the dependence of λ_l on $n^{(l+1)}$, $n^{(l+2)}$, ... we can substitute $n^{(j)} = \delta_{jl}$ for $j \leq l$ in both expressions, obtaining

$$\lambda_1 = 1 + 2n^{(2)} + 4n^{(3)} + ..., \qquad \lambda_2 = 2 + 4n^{(3)} + 8n^{(4)} + ...,$$

$$\lambda_k = 2^{k-1} + \sum_{j=1}^{\infty} 2^{k+j-1} n^{(k+j)}, \qquad (4.46)$$

for $l = 1$, 2, and any value of k. By combining (4.46) with (4.44), *we obtain explicit expressions for the boson creation matrices in terms of fermionic creation and annihilation matrices* $\bar{c}_j$ and c_j *affecting the bosonic quantal tape.* Again because the eigenvalues $n_l^{(k+j)}$ of the $n^{(k+j)}$ are all zero beyond a certain value of j, only a finite number of terms in the infinite series for λ_k is significant and the remaining qubits of the infinite tape are not used.

*The relations (4.40) are both satisfied by (4.44) and (4.46). The binary expansion of the matrix $N+1$ corresponding to (4.42) is an implicit analogue of the algorithm used on electronic computers, and given by

$$N + 1 = \sum_{j=1}^{\infty} 2^{j-1}(n^{(j)} + p^{(j-1)} - 2p^{(j)}),$$

$$p^{(0)} = 1, \qquad p^{(j)} = \prod_{k=1}^{j} n^{(k)} \qquad (j > 0).$$

4.4.3 Systems of Bosons

In quantized field theory it is necessary to represent the number and creation and annihilation operators for bosons in all possible states. The number of particles $N^{(r)}$ in the r-th state can be expressed in terms of the idempotents $n^{(r,j)}$ representing a countably inifnite set of qubits:

$$N^{(r)} = \sum_{j=1}^{\infty} 2^{j-1} n^{(r,j)}, \qquad (4.47)$$

or, alternatively, as for fermions, in terms of the creation and annihilation matrices defined by

$$N^{(1)} = \bar{b}_1 b_1 = N \otimes 1 \otimes 1..., \qquad \bar{b}_1 = \bar{b} \otimes 1 \otimes 1..., \qquad b_1 = b \otimes 1 \otimes 1...,$$

$$N^{(2)} = \bar{b}_2 b_2 = 1 \otimes N \otimes 1..., \qquad \bar{b}_2 = 1 \otimes \bar{b} \otimes 1..., \qquad b_2 = 1 \otimes b \otimes 1...,$$

$$N^{(3)} = \bar{b}_3 b_3 = 1 \otimes 1 \otimes N..., \qquad \bar{b}_3 = 1 \otimes 1 \otimes \bar{b}..., \qquad b_3 = b \otimes 1 \otimes 1..., \qquad (4.48)$$

etc.; no factors such as the $\xi^{(s)}$ in (4.38) are necessary, since these boson creation and annihilation operators satisfy *commutation relations* instead of anti-commutation relations:

$$[b_r, \bar{b}_s] \equiv b_r\bar{b}_s - \bar{b}_s b_r = \delta_{rs}, \qquad b_r b_s = b_s b_r, \qquad \bar{b}_r\bar{b}_s = \bar{b}_s\bar{b}_r. \qquad (4.49)$$

4.5 Observables with Continuous Spectra

The observables considered so far in the present chapter and the previous two chapters of this book have had *discrete* eigenvalues, usually integers or half-integers, separated by finite intervals within which no measured value of the observable could fall.

In terms of the boson creation and annihilation matrices $\bar{b}$ and b, and the unit μ of momentum,

$$q = \tfrac{1}{2}\hbar(b + \bar{b})/\mu, \qquad p = \mathrm{i}\mu(\bar{b} - b). \qquad (4.50)$$

These matrices are both hermitean and, since $c\bar{c} - \bar{c}c = 1$, we have

$$qp - pq = \mathrm{i}\hbar. \qquad (4.51)$$

This is the matrix relation first introduced by Born and Jordan, connecting a canonical coordinate observable q and its conjugate momentum observable p. It is easily seen that there can be no finite representation of q and p, for in any such representation the trace of $qp - pq$ would vanish, whereas the trace of the right side of (4.50) does not vanish. However, there are infinite representations, in which $\mathrm{tr}(qp)$ and $\mathrm{tr}(pq)$ are both infinite. Elements of

countably infinite matrices representing q and p are given explicitly in Sect. A.5, and it is shown there that they may have as an eigenvalue any real number. *Their spectra are therefore continuous.*

There is an obvious generalization of (4.50) and (4.51) for the construction any number of canonically conjugate coordinate and momentum observables $q^{(r)}$ and $p^{(r)}$ in terms of the boson creation and annihilation matrices $\bar{b}_r$ and b_r of (4.49):

$$q^{(r)} = \tfrac{1}{2}\hbar(b_r + \bar{b}_r)/\mu_r, \qquad p^{(r)} = \mu_r(\bar{b}_r - b_r). \tag{4.52}$$

From (4.49) it then follows that

$$q^{(r)}p^{(s)} - p^{(s)}q^{(r)} = \mathrm{i}\hbar\delta_{rs}. \tag{4.53}$$

4.5.1 Quasi-continuous Spectra

The countably infinite representations considered in Sect. A.5 suffer from the disadvantage that neither of the matrices representing p and q can be diagonalized, since the diagonal elements of any matrix in those representations can be numbered 1, 2, 3, ..., whereas the eigenvalues of an observable a with a continuous spectrum cannot be counted in this way.

However, for any experimental detector of such an observable there is in fact always a limit L to the number of significant binary fractional digits of the measured value, and there is also a finite lower limit a_{-M} to the measured values, so that it is both possible and meaningful to represent the observable in the form

$$a = a_{-M} + \sum_{j=-L}^{\infty} 2^{j-1} n^{(j)}, \tag{4.54}$$

similar to (4.42), again on the understanding that only a finite number of the countably infinite projections $n^{(j)}$ $(j = -L, \ldots\infty)$ will have the non-vanishing eigenvalue $n_1^{(j)} = 1$. The lower limit a_{-M} may be negative, positive or zero, but if L is sufficiently large the spectrum of the observable may be described as 'quasi-continuous'. Again the elements $n^{(j)}$ can be factorized in the same way as for fermions:

$$n^{(j)} = \bar{c}_j c_j = 1 - c_j\bar{c}_j, \qquad \bar{c}_j^2 = c_j^2 = 0. \tag{4.55}$$

With a finite value of L, the analogue of (4.44) is

$$\bar{c} = \lambda_{-L}^{\frac{1}{2}}\bar{c}_{-L} + \lambda_{-L+1}^{\frac{1}{2}}c_{-L}\bar{c}_{-L+1} + \lambda_{-L+2}^{\frac{1}{2}}c_{-L}c_{-L+1}\bar{c}_{-L+2} + \ldots,$$

$$\mathrm{c} = \lambda_{-L}^{\frac{1}{2}}c_{-L} + \lambda_{-L+1}^{\frac{1}{2}}c_{-L+1}\bar{c}_{-L} + \lambda_{-L+2}^{\frac{1}{2}}c_{-L+2}\bar{c}_{-L+1}\bar{c}_{-L} + \ldots, \tag{4.56}$$

where again the coefficients $\lambda_k^{\frac{1}{2}}$ depend only on the $n^{(j)}$ with $j > k$, and are given by

$$\lambda_k = 2^{k-1} + \sum_{j=1}^{\infty} 2^{k+j-1} n^{(k+j)}, \tag{4.57}$$

From (4.55) it follows that

$$\bar{c}c = \lambda_{-L}n^{(-L)} + \lambda_{-L+1}n^{(-L+1)}(1 - n^{(-L)}) + \ldots = a - a_{-M},$$

$$\bar{c}c = \lambda_{-L}(1-n^{(-L)}) + \lambda_{-L+1}(1-n^{(-L+1)})n^{(-L)} + \ldots = a - a_{-M} + 2^{-L} \tag{4.58}$$

and the renormalized bosonic commutation relation is now

$$c\bar{c} - \bar{c}c = 2^{-L-1}. \tag{4.59}$$

The difference between successive eigenvalues of $\bar{c}c$ is therefore 2^{-L-1}, and can be made to correspond to the degree of accuracy of any experimental measurement of a.

4.6 Summary

This chapter extends to a variety of other physical applications the possibility of an informationally based description in terms of qubits. The introductory applications are to the formulation of an equation of a rather general type for the description of particles with spin greater than one half and its application to Maxwell's equations for the description of electromagnetic phenomena, which it is shown, can be formulated as an equation for the photon of the same type as for other elementary particles, with an interpretation in terms of qubits. Further applications are made to systems of fermions and bosons, the two fundamental constituents of matter, and to the possibility of representing the results of measurement of even those observables with a theoretical continuum of measurable values in terms of qubits.

5. Observables and Information

The discovery of quantum mechanics was made in 1925, and the statistical interpretation of quantum mechanics which came to be generally accepted was made by Born in 1926. At that time Born pointed out, however, that uncertainty in quantum mechanics had implications that were quite different from those in already existing branches of statistical physics. Since information theory was not developed until 1949, however, the nature of this distinction remained unclear for some time, and has received little attention in much of the subsequent literature. Consequently, various attempts to restore the determinism of Newtonian physics have proliferated; they include the theory of the universal wave function, the theory of hidden variables, and the 'many worlds' interpretation of quantum mechanics. In general these theories require the existence of a multiplicity of phenomena that are unobservable; they do not represent information to be gained; and therefore will not receive consideration in the present context. In this chapter we shall give a general account of quantum mechanics in a form which is consistent with quantal information theory and which provides the underlying reasons why such imaginative attempts to model phenomena that are, as far as is known, unpredictable have not been rewarded.

The physical systems to be considered may be 'microscopic', by which we usually mean sub-microscopic and consisting of a relatively small number of particles, or macroscopic and amenable to direct observation. The distinction between them is made more precise by noting that information concerning a microscopic system can only be gained by allowing the system to interact with a macroscopic system which is sufficiently sensitive to be palpably affected by the interaction. The information gained depends of course not only on the apparatus employed to detect the system, but on the state of the system. The apparatus determines the observable or observables concerning which information is gained, and the state of the system determines the information gained, or more precisely the probability of any outcome of the observation. In the last three chapters we have been concerned mainly with the description, or representation, of the observables, but our next aim is to determine their eigenvalues, which are the possible results of their observation, and also to represent the state of the system by a statistical matrix which determines the probability that a particular result will be observed.

We have already seen how the representation of the number of fermions or bosons of a particular kind, and their dynamical observables can be expressed in terms of qubits. The dynamical observables of a particle of spin S, its energy, momentum, spin angular momentum and central vector, have been identified as the generators α_{jk} of the de Sitter group in a particular representation, where the subscipts j and k take values 0, 1, 2, 3, or 4, and satisfy the commutation relations given in (4.17). Any microscopic or macroscopic system is made up of different particles of these types, and as the dynamical observables are additive, the commutation relations are the same for the composite system as for its constituents. In the context of information theory, the entire system has a representation as a set of qubits on a quantal 'tape' with components representing contributions from individual particles of the kind already considered.

The first three sections of this chapter will be concerned with nonrelativistic and special relativistic quantum mechanics, where the commutation rules are not those of the de Sitter group, but well defined approximations to them which are extremely good in many applications. But we shall begin by stating the exact commutation relations for a general system consisting of N particles. We note that for such a system the fundamental observables may be represented in terms of direct products with N factors, thus:

$$A_{jk} = \alpha^{(1)}_{jk} + \alpha^{(2)}_{jk} + \ldots \alpha^{(N)}_{jk}, \qquad \alpha^{(1)}_{jk} = \alpha^{[1]}_{jk} \otimes 1 \ldots \otimes 1, \qquad \alpha^{(2)}_{jk} = 1 \otimes \alpha^{[2]}_{jk} \ldots \otimes 1 \ldots,$$

$$\alpha^{(N)}_{jk} = 1 \otimes 1 \ldots \otimes \alpha^{[N]}_{jk}. \tag{5.1}$$

where the factor $\alpha^{[a]}_{jk}$ has the same form as α_{jk} in (4.17), but is for the a-th particle, with a spin $S^{[a]}$ depending on the type of particle. In this general context, the A_{jk} are still generators of an extended de Sitter group $SO(5,1)$, and also the elements of its Lie algebra $so(5,1)$; in fact it follows from (5.1) that they satisfy the same relations

$$[A_{jk}, A_{lm}] \equiv A_{jk}A_{lm} - A_{lm}A_{jk} = g_{kl}A_{jm} - g_{jl}A_{km} - g_{km}A_{jl} + g_{jm}A_{kl}. \tag{5.2}$$

as the $\alpha^{[a]}_{jk}$, or α_{jk} in (4.17). The elements $\mathrm{i}A_{12}$ and A_{34} of the algebra commute, and as components of the angular momentum and momentum, are in the same x_3-direction.

In the quantum mechanics of charged particles, it is usually sufficient to restrict the subscripts to values not greater than 4, and the resulting subalgebra is then the de Sitter algebra $so(4,1)$, whose structure we shall now consider. As pointed out in more detail in Sect. A.6, the representations of a Lie algebra, such as the de Sitter algebra, are in correspondence with the eigenvalues of the matrices called its invariants, which commute with all elements of the algebra. In an irreducible representation the invariants serve to identify the representation and are numerical multiples of the unit matrix,

while in a reducible representation they are diagonal matrices with eigenvalues that serve to identify the irreducible representations which it contains. There are various invariants of the Lie algebra $so(4,1)$ of the de Sitter group, but only two of them are independent and they can be chosen in different ways. In any irreducible representation we shall regard as fundamental the *highest weights* $J_{\max}$ and $K_{\max}$ defined so that if $2\pi\hbar$ as usual is Planck's constant and c is the velocity of light,

(a) the maximum eigenvalue of the component J_3 of the angular momentum $\mathbf{J} = \mathrm{i}(A_{23}, A_{31}, A_{12})$ of the system (in units of $\hbar$) is $J_{\max}$. This normally has contributions from the orbital motions as well as from the spins of the constituent particles.

(b) the maximum eigenvalue of the component K_3 of the momentum $\mathbf{K} = (A_{14}, A_{24}, A_{34})/R$ (in units of $\hbar$, if R is th radius of de Sitter space), when J_3 already has the eigenvalue $J_{\max}$, is $K_{\max}$.

The invariants of certain subalgebras of $so(4,1)$ have a even more direct physical significance. Of special importance are the invariants $-\frac{1}{2}A^{\lambda}_{\mu}A^{\mu}_{\lambda}$ (with implied summation over $\lambda, \mu = 0, 1, 2, 3$) of the Lorentz subalgebra $so(3,1)$, and $-\frac{1}{2}A^{\alpha}_{\beta}A^{\beta}_{\alpha}$ ((with implied summation over $\alpha, \beta = 1, 2, 3$) of its rotation subalgebra $so(3)$, whose elements have been identified as cartesian components of the angular momentum $\mathbf{J}$ of the system (again in units of $\hbar$) in a particular state. There is a further invariant

$$M^2c^2R^2 = \tfrac{1}{2}\hbar^2(A^{\lambda}_{\mu}A^{\mu}_{\lambda} - A^{j}_{k}A^{k}_{j}) = -\hbar^2 A^{j}_{4}A^{4}_{j}, \tag{5.3}$$

of the Lorentz group which is of great physical importance since, when R is the radius of the de Sitter space, it determines the mass M of the system. For a system consisting of a single particle, this is the rest-mass, but in general it includes a contribution from the energy of the constitutent particles.

The generators A_{jk} of the de Sitter group all have a physical interpretation. The energy E, and the cartesian components of the momentum $\mathbf{K}$, the angular momentum $\mathbf{J}$, and the central vector $\mathbf{C} = M\mathbf{X}$ (where M is the mass as defined above, and $\mathbf{X}$ is then interpreted as the position vector of the centre of mass) of the system are

$$E = \hbar c A_{04}/R, \qquad (K_1, K_2, K_3) = \hbar(A_{14}, A_{24}, A_{34})/R$$

$$(J_1, J_2, J_3) = \mathrm{i}\hbar(A_{23}, A_{31}, A_{12}), \qquad (C_1, C_2, C_3) = \hbar(A_{01}, A_{02}, A_{03})/c. \tag{5.4}$$

In detail, the relations (5.1) are then

$$[K_\alpha, E] = -\mathrm{i}c\hbar C_\alpha/R^2, \qquad [J_\alpha, E] = 0, \qquad [C_a, E] = \mathrm{i}\hbar K_\alpha,$$

$$[K_\alpha, K_\beta] = \mathrm{i}h\sum_\gamma \epsilon_{\alpha\beta\gamma}J_\gamma/R^2, \qquad [J_\alpha, K_\beta] = \mathrm{i}h\sum_\gamma \epsilon_{\alpha\beta\gamma}K_\gamma,$$

$$[C_\alpha, K_\beta] = \mathrm{i}\hbar\delta_{\alpha\beta}E/c^2, \qquad [J_\alpha, J_\beta] = \mathrm{i}\hbar\sum_\gamma \epsilon_{\alpha\beta\gamma}J_\gamma,$$

$$[C_\alpha, J_\beta] = \mathrm{i}\hbar \sum_\gamma \epsilon_{\alpha\beta\gamma} C_\gamma, \qquad [C_\alpha, C_\beta] = -\mathrm{i}\hbar \sum_\gamma \epsilon_{\alpha\beta\gamma} J_\gamma / c^2. \tag{5.5}$$

According to (5.3), the mass is of the system then given by $M^2c^2 = E^2/c^2 - \mathbf{K}^2$, and we have the relativistic relation

$$E/c = (M^2c^2 + \mathbf{K}^2)^{\frac{1}{2}} \tag{5.6}$$

between energy, mass and momentum.

5.1 Relativistic and Non-relativistic Approximations

From (5.3), it is clear that there are two useful approximations to the commutation rules:

(1) Except in the cosmological context, the factor $1/R^2 \sim 10^{-54}$ cm^{-2} is quite negligible, so that it may be assumed that the components $(E/c, K_1, K_2, K_3)$ of the energy–momentum four-vector of the system commute with one another: $[K_\alpha, E] = [K_\alpha, K_\beta] = 0$. The resulting commutation rules are then those of the Poincaré group, in common use in conjunction with the special theory of relativity, and will be used in Sect. 5.3.

(2) In a non-relativistic context, all observables are assumed to be hermitean. The velocity of light c is very large compared with the velocity $|\mathbf{K}|/M$ of the system, so that (5.4) may be approximated by

$$E = Mc^2 + \mathbf{K}^2/(2M). \tag{5.7}$$

The first term on the right side is the *rest energy* predicted by Einstein on the basis of his special theory of relativity and for a non-relativistic system is very much greater than second term, which is the *kinetic energy* of the system Thus, when (5.4) is substituted into the sixth of the commutation relations of (5.5), the contribution of the second term to the right side is quite negligible and this commutation relation reduces to $[C_\alpha, K_\beta] = \mathrm{i}\hbar\delta_{\alpha\beta}M$, or

$$[X_\alpha, K_\beta] = \mathrm{i}\hbar\delta_{\alpha\beta}, \qquad X_\alpha = C_\alpha/M, \tag{5.8}$$

when the cartesian position vector $\mathbf{X}$ of the system is defined by $\mathbf{C} = M\mathbf{X}$ as in the classically compatible theory of Sect. 1.2.

The above commutation relations are consistent with those already obtained for canonically conjugate coordinate and momentum observables in (4.53). As in the special relativistic approximation, different components of the momentum vector $\mathbf{K}$ commmute with one another, and because the velocity of light c is so much greater than other observed velocities, the right side of the last of the commutation relations can be neglected, so that

$$[K_\alpha, K_\beta] = [X_\alpha, X_\beta] = 0. \tag{5.9}$$

Much of non-relativistic quantum mechanics of an isolated system S is based on the relations (5.8) and (5.9), in conjunction with the formula (5.7) for the energy. Where the system is composite, consisting of a number of interacting sub-systems $\mathrm{S}^{(r)}$ $(r = 1, 2, ...)$, the rest energy Mc^2 must be considered to include the relatively small interaction energy V of the sub-systems, depending only on their relative coordinates which commute with all the fundamental observables of the system S. When the sub-systems are particles with coordinates $\mathbf{x}^{(r)}$ and momenta $\mathbf{k}^{(r)}$ $(r = 1, 2...)$, we make use of the commutation relations

$$[x_\alpha^{(r)}, k_\beta^{(s)}] = \mathrm{i}\hbar\delta_{\alpha\beta}\delta_{rs}, \qquad [k_\alpha^{(r)}, k_\beta^{(s)}] = [x_\alpha^{(r)}, x_\beta^{(s)}] = 0. \tag{5.10}$$

We shall consider next a few examples of the application of these ideas.

5.1.1 Orbital Angular Momentum

The angular momentum $\mathbf{J}$ in (5.5) includes both the spin angular momentum $\mathbf{S}$ and the orbital angular momentum $\mathbf{L}$ of the system. To separate these two components, in the context of non-relativistic quantum mechanics we introduce an independent definition of the orbital angular momentum $\mathbf{L}$ which is essentially that of Newtonian mechanics. The spin angular momentum will then be $\mathbf{S} = \mathbf{J} - \mathbf{L}$.

In terms of the vectors $\mathbf{X}$ and $\mathbf{K}$ or their components,

$$\mathbf{L} = \mathbf{X} \times \mathbf{K}, \qquad L_\alpha = \sum_{\beta,\gamma} \epsilon_{\alpha\beta\gamma} X_\beta K_\gamma. \tag{5.11}$$

It is important that, with this defintion, the orbital angular momentum satisfies the same commutation relations with other observables as $\mathbf{J}$ in (5.5), and we therefore verify with the help of (5.8) and (5.9).that

$$[L_1, L_2] = [X_2P_3 - X_3P_2, X_3P_1 - X_1P_3] = \mathrm{i}\hbar(X_1P_2 - X_2P_1) = \mathrm{i}\hbar L_3,$$

so, by cyclic permutation of affixes,

$$[L_\alpha, L_\beta] = \mathrm{i}\hbar \sum_\gamma \epsilon_{\alpha\beta\gamma} L_\gamma; \tag{5.12}$$

also,

$$[L_a, X_\beta] = [\sum_{\rho,\sigma} \epsilon_{\alpha\rho\sigma} X_\rho K_\sigma, X_\beta] = -\mathrm{i}\hbar \sum_{\rho,\sigma} \epsilon_{\alpha\rho\sigma} X_\rho \delta_{\sigma\beta} = \mathrm{i}\hbar \sum_\rho \epsilon_{\alpha\beta\rho} X_\rho,$$

$$[L_a, K_\beta] = [\sum_{\rho,\sigma} \epsilon_{\alpha\rho\sigma} X_\rho K_\sigma, K_\beta] = \mathrm{i}\hbar \sum_{\rho,\sigma} \epsilon_{\alpha\rho\sigma} K_\sigma \delta_{\rho\beta} = \mathrm{i}\hbar \sum_\sigma \epsilon_{\alpha\beta\sigma} K_\sigma.$$

Moreover, $\mathbf{L}$ commutes with all scalars formed from the vectors $\mathbf{X}$, $\mathbf{K}$ and $\mathbf{L}$, e.g.,

$$[L_1, \mathbf{X}\cdot\mathbf{K}] = [L_1, X_1K_1 + X_2K_2 + X_3K_3]$$
$$= \mathrm{i}\hbar(X_3K_2 + X_2K_3 - X_2K_3 - X_3K_2) = 0.$$

Another important identity reminiscent of Newtonian mechanics connects the scalars $\mathbf{L}^2$, $\mathbf{K}^2$, $\mathbf{X}^2$ and $\mathbf{X}\cdot\mathbf{K}$. By cyclic permutation of affixes in the identity

$$(X_2K_3 - X_3K_2)^2 = X_1^2K_1^2 + X_2^2K_3^2 + X_3^2K_2^2$$
$$-X_1(K_1X_1 + \mathrm{i}\hbar)K_1 - 2X_2K_2X_3K_3 + \mathrm{i}\hbar(X_2K_2 + X_3K_3)$$

and by addition of the results we have

$$\mathbf{L}^2 = \mathbf{X}^2\mathbf{K}^2 - \mathbf{X}\cdot\mathbf{K}(\mathbf{X}\cdot\mathbf{K} - \mathrm{i}\hbar). \tag{5.12}$$

From (5.12) it is evident that, like the J_α, the components L_α of the orbital angular momentum are elements of the Lie algebra $so(3)$ of the group of rotations. The quadratic invariant I of this algebra is $\mathbf{L}^2$, and from the result of (A.72) it follows that the eigenvalue of $\mathbf{L}^2$ in an irreducible representation is $L(L+1)\hbar^2$, if $L\hbar$ is the maximum eigenvalue of L_3 in the representation. This result may be confirmed very simply in this instance, as follows. If g_I is the eigenmatrix of L_3 corresponding to the eigenvalue L_{3I} of L_3, we have

$$L_3(L_1 + \mathrm{i}L_2)g_I = (L_1 + \mathrm{i}L_2)(L_3 + \hbar)g_I = (L_{3I} + \hbar)(L_1 + \mathrm{i}L_2)g_I,$$

so that in general $(L_{3I} + \hbar)$ is also an eigenvalue. But if g_I is the eigenmatrix corresponding to the maximum eigenvalue $L\hbar$, there is no eigenvalue $(L_{3I}+\hbar)$ of L_3, so that $(L_1 + \mathrm{i}L_2)g_I$ must be zero. From this it follows that

$$\mathbf{L}^2 g_I = [(L_1 - \mathrm{i}L_2)(L_1 + \mathrm{i}L_2) + L_3(L_3 + \hbar)]g_I = L(L+1)\hbar^2 g_I.$$

The eigenvalues of L_3 differ by integral multiples of $\hbar$, and since $\mathbf{K}\cdot\mathbf{L} = 0$, where $\mathbf{K}$ may have any direction, it is evident that 0 must be an eigenvalue, and that L must always be an integer. In contrast, as we have already seen, the maximum eigenvalue $S\hbar$ of a component S_3 of the spin angular momentum may be an integer *or* a half-integral multiple of $\hbar$.

5.2 Non-relativistic Quantum Mechanics

In the period leading up to and immediately following the first formulations of quantum mechanics, much effort was devoted to the understanding of *atomic spectra*. Following the experimental investigations of Rutherford and others, it was realized that neutral atoms consisted of a nucleus carrying a positive electric charge, and a compensating negative charge associated with a fixed number (the atomic number) of electrons which determined the chemical properties of the atom. It was not easy to explain the undoubted stability of such a system on the basis of the classical theories of electricity, but this

was clearly connected with the fact that atoms were able to absorb and emit energy in the form of radiation with fixed frequencies. The simplest example was in the emission or absorption of electromagnetic radiation by hydrogen, where the observed angular frequencies $\omega_{\nu\nu'}$ were related, by the *Balmer formula* $B_\nu - B_{\nu'} = \hbar\omega_{\nu\nu'}$ to differences in discrete binding energies B_ν and $B_{\nu'}$ of the electron before and after emission or absorption. According to Bohr's precursor of quantum theory, the energy levels B_ν $(\nu = 1, 2, ...)$ for hydrogen were given, to a good approximation, by the relatively simple formula

$$B_\nu = -\tfrac{1}{2}mc^2\alpha^2/\nu^2 \qquad [\alpha = e^2/(4\pi\hbar c) \approx 1/137.036], \tag{5.13}$$

where the coeffcient $\frac{1}{2}mc^2\alpha^2/\hbar^2$ was related to the wave number $mc^2\alpha^2/(4\pi c\hbar)$, which had been identified in spectroscopy as the Rydberg constant. The dimensionless constant α is now known as the *fine-structure constant*. For hydrogen-like atoms with a nuclear charge of Ze, the binding energy of an electron to the nucleus was $-\frac{1}{2}Z^2mc^2\alpha^2/\nu^2$, or $-Z^2e^2/(8\pi a_B\nu^2)$ in terms of the Bohr radius $a_B = \hbar/(mc\alpha)$.

Other simple but important applications of non-relativistic quantum mechanics are to the scattering of one particle by another, and were first treated by Born in an application of perturbation theory to Schrödinger's wave mechanics. Perhaps in consequence, wave-mechanical methods were at first generally used to calculate the differential and total cross-sections for the scattering of one microscopic particle by another. Later, simple and effective matrix methods were developed by Heisenberg and others for applications of this type, and the time-independent methods based on the theory of the S-matrix will also be considered in this section. In some applications, for instance in the electrostatic scattering of one charged particle by another, the results do not differ appreciably from those obtained on the basis of classical mechanics, except at low energies where Planck's constant $\hbar$ has a significant role in the formula for the cross-sections. But with short-range forces, the quantal effects were evident even at high energies, where relativistic effects also become important. A relativistic analysis of scattering problems requires the use of field theoretical methods, to be discussed in the next chapter, and of the statistical matrix, the theory of which will be developed later in the present chapter.

5.2.1 The Hydrogen Atom

To obtain Bohr's result (5.13) on the basis of non-relativistic quantum mechanics, we consider a composite system, such as a hydrogen atom, consisting of two particles, such as a proton and an electron, whose coordinate and momentum observables will be denoted by $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ and $\mathbf{k}^{(1)}$ and $\mathbf{k}^{(2)}$ respectively. If $m^{(1)}$ and $m^{(2)}$ are the masses of the particles, the energy E of the system, excluding the rest energies of the particles is the sum of their kinetic energies and their energy V of interaction:

$$E = \mathbf{k}^{(1)2}/2m^{(1)} + \mathbf{k}^{(2)2}/2m^{(2)} + V(\mathbf{r}), \qquad \mathbf{r} = \mathbf{x}^{(2)} - \mathbf{x}^{(1)}. \tag{5.14}$$

As in Newtonian mechanics, the kinetic energy is separated into the kinetic energy $\mathbf{K}^2/2M$ of the centre of mass and the kinetic energy $\mathbf{p}^2/2m$ of the relative motion, which can be expressed in terms of the relative velocity $\mathbf{k}^{(2)}/m^{(2)} - \mathbf{k}^{(1)}/m^{(1)}$ and the *reduced mass* m, thus:

$$E = \mathbf{K}^2/2M + \mathbf{k}^2/2m + V(\mathbf{r}),$$
$$\mathbf{K} = \mathbf{k}^{(1)} + \mathbf{k}^{(2)}, \qquad \mathbf{k} = m(\mathbf{k}^{(2)}/m^{(2)} - \mathbf{k}^{(1)}/m^{(1)}),$$
$$M = m^{(1)} + m^{(2)}, \qquad m = m^{(1)}m^{(2)}/M. \tag{5.15}$$

As a consequence of the commutation relations (5.10),

$$[r_\alpha, k_\beta] = \mathrm{i}\hbar\delta_{\alpha\beta}, \qquad [k_\alpha, k_\beta] = [r_\alpha, r_\beta] = 0.$$

The kinetic energy $\mathbf{K}^2/2M$ of the motion of the centre of mass has a continuous spectrum, and its eigenvalue can be reduced to zero by the choice of an inertial frame in which $\mathbf{K} = 0$. The effects of most interest are therefore those resulting from the quantization of the observables of the relative motion. For the hydrogen-like atom with a nuclear charge Ze, the important contribution to the interaction energy $V(\mathbf{r})$ between the nucleus and an electron is the electrostatic attraction $-Ze^2/(4\pi r)$, where $r = |\,\mathbf{r}\,|$ is the distance between the proton and the electron, so that the energy of the relative motion is

$$B = \mathbf{k}^2/2m - Z\alpha\hbar c/r, \qquad [\alpha = e^2/(4\pi\hbar c)]. \tag{5.16}$$

To find the eigenvalues of this observable, we first separate the angular and radial contribitions to the kinetic energy $\mathbf{k}^2/2m$. This can be done by making use of the result of (5.12), which in this application yields

$$\mathbf{l}^2/r^2 = \mathbf{k}^2 - r^{-2}\mathbf{r}\cdot\mathbf{k}(\mathbf{r}\cdot\mathbf{k} - \mathrm{i}\hbar) = \mathbf{k}^2 - k_r^2, \qquad k_r = r^{-1}(\mathbf{r}\cdot\mathbf{k} - \mathrm{i}\hbar),$$

since $r^{-1}\mathbf{r}\cdot\mathbf{k} = (\mathbf{r}\cdot\mathbf{k} - \mathrm{i}h)r^{-1}$. In spite of appearances, the radial component k_r of the momentum defined in this way is hermitean, and together with the radial coordinate r satisfies the usual canonical commutation relation

$$rk_r - k_r r = \mathrm{i}\hbar. \tag{5.17}$$

In terms of these, the formula (5.16) for the binding energy can be written

$$2mB = k_r^2 + l(l+1)\hbar^2/r^2 - 2Zm\alpha\hbar c/r, \qquad l(l+1)\hbar^2 = \mathbf{l}^2, \tag{5.18}$$

where, according to the discussion following (5.12), the eigenvalues of l are positive integers.

The eigenvalues of $2mB$ can now be found by a straightforward application of the factorization method. If B_1 is the least eigenvalue of B, in

accordance with (A.43) $2m(B - B_1)$ can be factorized in the form $\bar{c}_1 c_1$, and successive eigenvalues B_ν of B are then given in increasing order by

$$2mB = \bar{c}_1 c_1 + 2mB_1, \qquad \bar{c}_{\nu+1}c_{\nu+1} + 2mB_{\nu+1} = c_\nu\bar{c}_\nu + 2mB_\nu \qquad (\nu = 1, 2, \ldots), \tag{5.19}$$

where $\bar{c}_\nu$ is the hermitean conjugate of c_ν. In this instance the factors c_ν and $\bar{c}_\nu$ must clearly be of the form

$$c_\nu = k_r + \mathrm{i}(\alpha_\nu + \beta_\nu/r), \qquad \bar{c}_\nu = k_r - \mathrm{i}(\alpha_\nu + \beta_\nu/r),$$

so that

$$\bar{c}_\nu c_\nu = k_r^2 + (\alpha_\nu + \beta_\nu/r)^2 - \beta_\nu\hbar/r^2, \qquad c_\nu\bar{c}_\nu = k_r^2 + (\alpha_\nu + \beta_\nu/r)^2 + \beta_\nu\hbar/r^2.$$

By substitution from (5.19), with the help of (5.18) we have $\beta_1 = (l+1)\hbar$ and

$$2mB_\nu = -\alpha_\nu^2, \qquad \alpha_\nu\beta_\nu = mZe^2, \qquad \beta_{\nu+1}(\beta_{\nu+1} - \hbar) = \beta_\nu(\beta_\nu + \hbar). \tag{5.20}$$

Hence $\beta_\nu = (l+\nu)\hbar$, $\alpha_\nu = mZe^2/[4\pi\hbar(l+\nu)]$ and

$$B_\nu = -mZ^2e^4/[32\pi^2\hbar^2(l+\nu)^2]. \tag{5.21}$$

This result, obtained by Pauli on the basis of the matrix formulation of quantum mechanics and by Schrödinger on the basis of his wave mechanics, is obviously in agreement with (5.13) for $Z = 1$ and s-states for which $l = 0$, but predicts also that for $l > 0$ the energy levels are *degenerate*, in the sense that two or more energy levels coincide. Experimentally it is found that the formula (5.21) represents a good approximation to what is observed, but, instead of coinciding, the 'degenerate' levels, though very close together, are separated by an amount depending on the fine-structure constant $\simeq 1/137.036$. It was soon realized that it was necessary to take account of the spin of the electron to account for the multiplet structure of the energy levels of the hydrogen atom, but a satisfactory explanation of the fine structure had to await Dirac's special relativistic theory of the electron, to be considered in Sect. 5.4 below. There is still another degeneracy of the spectrum of the hydrogen atom, associated with the $2l+1$ different eigenvalues of a component l_3 (with a suitable choice of the coordinate axes) of the angular momentum $\mathbf{l}$. This degeneracy accounts for the *Zeeman effect*, a splitting of the spectral lines of the hydrogen atom in a magnetic field which had already been observed near the end of the nineteenth century.

*Unlike an electron and a proton, a neutron and a proton have only one bound state, the deuteron, predominantly in an s-state ($l = 0$). Their interaction energy is quite well represented by the Hulthén potential $-f/\rho$, where $\rho = (\mathrm{e}^{\mu r} - 1)/\mu$ and μ is the meson mass. By choosing c_1 to be of the form $k_r + \mathrm{i}(\alpha - \beta/\rho)$, the binding energy B of the deuteron is found to be given by

$$MB = -(\tfrac{1}{2}\mu\hbar - Mf/\hbar)^2,$$

where M is twice the reduced mass ($\sim$ the mass of a nucleon). Other eigenvalues can be obtained, but are positive and correspond to dissociated states of the deuteron.

It is a result of the theory of the factorization method given in Sect. A.4 that the eigenmatrices g_k of the energy, corresponding to the eigenvalues B_ν, are simply related to one another by the factors c_k and $\bar{c}_\nu$ of (5.19): if $\nu > 1$ then $c_\nu g_\nu = g_{\nu-1}c_\nu$ and $\bar{c}_\nu g_{\nu-1} = g_\nu \bar{c}_\nu$. There is no eigenmatrix g_0 and for $\nu = 1$, these relations reduce to $c_1 g_1 = 0$ and $g_1 \bar{c}_1 = 0$. Thus the eigenmatrices are all determined by the conditions

$$c_1 g_1 = 0, \qquad g_{\nu+1} = (\bar{c}_\nu c_\nu)^{-1} \bar{c}_\nu g_\nu c_\nu. \tag{5.22}$$

The bound states of the hydrogen atom, with energy levels given by (5.20), form only part of the spectrum of a proton and its associated electron. If the atom absorbs energy greater than the binding energy, the atom is ionized, and the electron escapes, in much the same way as if had been scattered by the proton. Ionized states correspond to imaginary values of α_ν in (5.20), the positive imaginary values corresponding to positive, outgoing radial momenta of the electron. The spectrum of the ionized states is continuous, but may be converted into a finely spaced discrete spectrum by the addition of an oscillator potential $\gamma^2 r^2$, with an arbitarily small value of γ, to the energy as given by (5.16); the additional term ensures that in ionized states the electron cannot escape to infinity. To obtain a complete set of energy levels under these conditions we take

$$c_\nu = k_r + \mathrm{i}(\alpha_\nu + \beta_\nu/r - \gamma_\nu r), \qquad \bar{c}_\nu = k_r - \mathrm{i}(\alpha_\nu + \beta_\nu/r - \gamma_\nu r),$$

with $\gamma_1 = \gamma$. The expressions already obtained for α_ν and β_ν are unaffected by the additional potential, but the eigenvalues of the energy are given by

$$2mB_\nu = -\alpha_\nu^2 + (2\beta_\nu + \hbar)\gamma_\nu,$$

$$\alpha_\nu \beta_\nu = me^2, \qquad \beta_\nu = (l+\nu)\hbar, \qquad \alpha_\nu \gamma_\nu = \alpha_1 \gamma. \tag{5.23}$$

The energy levels, though very closely spaced in the region of ionization, now extend to infinity.

5.2.2 Scattering and the S-Matrix

Much experimental work has been devoted to the measurement of the differential and total cross-sections for the scattering of one microscopic system by another, and the information gained in this way has been both an impetus an an aid to the theoretical understanding of the underlying quantal processes. In this section we shall consider here only elastic scattering, where the incident and scattered particles are the same, and the separation of observables

associated with the centre of mass and the relative motion in (5.15) is still effective.

The cross-section for the scattering of one particle by another is a concept developed originally in the context of classical physics, where if b is the distance between the paths of colliding spherical particles, in an inertial frame in which the total momentum $\mathbf{K}$ is zero, the total cross-section is $\sigma = \pi b^2$. If b is expressed as a function $b(\cos\theta)$ of the cosine of the scattering angle, the differential cross-section is then $d\sigma = bb'd\Omega$, where $d\Omega = 2\pi \sin\theta d\theta$ is the small solid angle corresponding to scattering angles between θ and $\theta + d\theta$. For two particles with relative momentum $\mathbf{k}$ and angular momentum $\mathbf{l}$, $b^2 = \mathbf{l}^2/\mathbf{k}^2$, so that the cross-section can be obtained by expressing the angular momentum in terms of the scattering angle. In the electrostatic scattering of particles with charges $Z_1 e$ and $Z_2 e$, the hyperbolic trajectories are characterized by the relation $b = a\cot(\frac{1}{2}\theta)$ between b and the distance a of closest approach, and since the radial momentum is zero at that distance a is given by $Z_1 Z_2 e^2/(4\pi a) = \mathbf{k}^2 - \mathbf{l}^2/a^2$; the total cross-section is therefore $\pi a^2 \cot^2(\frac{1}{2}\theta)$, as found by Rutherford. The large predicted scattering through small angles is due to the long range of the Coulomb forces and is normally reduced by the 'shielding' of a charge by charge of the opposite sign.

In quantum mechanics the experimentally measured cross-section is usually the result of the scattering of a beam of similar incident particles by a set of similar scattering particles. It is therefore defined as the expectation value of the number of particles scattered per unit time, per scatterer, per unit flux density of incident particles. With one incident particle per unit volume, the flux density is simply the velocity relative to the scatterers. As in classical theory, the differential cross-section $d\sigma$ is the fraction of the total cross-section for which the incident particle is scattered into the solid angle $d\Omega$, but as the angular momentum observable does not commute with the relative momentum, there are contributions to the cross-section from all eigenvalues of $\mathbf{l}^2$.

The interpretation of the experimental work can be based on a calculation of the conditional probability p_{if}/p_i that, after the scattering of one particle by another, the system will be found with an eigenvalue $\mathbf{k}_f$ of the relative momentum $\mathbf{k}$ if initially it had the eigenvalue $\mathbf{k}_i$. According to (1.22) and (1.24), this is $p_{if} = \langle g_i g_f\rangle/\langle g_i\rangle$, where g_f is related to g_i by a unitary transformation:

$$g_f = S g_i S^\dagger, \qquad SS^\dagger = 1 \tag{5.24}$$

As emphasized by Heisenberg in introducing this approach to the theory of scattering, although the S-matrix defined by this relation is unitary rather than hermitean and therefore not an observable, its elements can be considered to be observable quantities. If all incident particles have the momentum $\mathbf{k}_i$ then $\langle g_i\rangle = 1$ and for different values of $\mathbf{k}_f$ the *transition probabilities*

$$p_{if} = \mathrm{tr}(g_i g_f) = \mathrm{tr}[(g_i S g_i)(g_i S g_i)^\dagger],$$

which are clearly non-negative, determine the differential cross-section, given by

$$d\sigma = \sum_{\mathbf{k}_f \text{ in } d\Omega} p_{if}, \qquad \text{or} \qquad d\sigma = \int_{d\Omega} p_{if} d^3k_f, \tag{5.25}$$

when the scattered states are continuous. Since p_{if} is unchanged under any rotation changing g_i to $g_i' = ug_iu^{-1}$ and g_f to $g_f' = ug_fu^{-1}$, where $u^{-1} = u^\dagger$, it can only depend on $k^2 = \mathbf{k}^2$ and $\mathbf{k}\cdot\mathbf{k}' = k^2\cos\theta$, where θ is the scattering angle; and we may set $d^3k_f = 2\pi k^2 \sin\theta d\theta$.

The S-matrix depends on the energy $k^2/2m$ of the relative motion and commutes with the angular momentum $\mathbf{l}$, so that it may be expressed in the form

$$S = \sum_l S_l g_l \tag{5.26}$$

The coefficients S_l are unitary matrices, which are easily constructed from the factors $\bar{c}_\nu$ and c_ν of (5.19). The unbound states require imaginary values of α_ν in (5.20), with negative imaginary values corresponding to incident momenta and positive imaginary values to scattered momenta. We therefore write

$$S_l = \prod_{r=1}^{\nu} [(k + \mathrm{i}\alpha_r)^{-1}] c_1 c_2 \ldots c_\nu. \tag{5.27}$$

and verify with the help of (A.46) and $k^2 + \alpha_r^2 = k^2 - 2mB_r$ that $S_l S_l^\dagger = 1$. The bound states correspond to poles $k^2 = -\alpha_r$ of the S-matrix, and usually the α_r decrease rapidly in absolute value with r, so that good approximations to the product in (5.27) are easy to calculate.

5.3 Uncertainty Relations

We shall now give a simple derivation of the general uncertainty relation between two observables already stated in (1.27). We consider two different observables a and b, represented by hermitean matrices which in general do not commute with one another, and write

$$[a, b] \equiv ab - ba = \mathrm{i}c, \tag{5.28}$$

so that $\mathrm{i}c$ is the *commutator* of a and b. The hermitean conjugate of ab is ba, so that the hermitean conjugate of $[a, b]$ is $-[a, b]$. As the hermitean conjugate of i is $-\mathrm{i}$, c must be hermitean and is an observable. The deviations δa and δb of a and b from their expectation values $\langle a\rangle$ and $\langle b\rangle$ are matrices given by

$$\delta a = a - \langle a\rangle, \qquad \delta b = b - \langle b\rangle, \tag{5.29}$$

where, as usual in matrix equations, $\langle a\rangle$ and $\langle b\rangle$ are intepreted as corresponding numerical multiples of the unit matrix. According to (1.18) and (5.29) the uncertainty Δa in a and b are given by

$$\Delta a^2 = \langle \delta a^2\rangle = \sum_s \widetilde{p}_s \mathrm{tr}(\widetilde{g}_s \delta a^2), \tag{5.30}$$

*Since $\mathrm{tr}(\widetilde{g}_s^2 \delta a^2) = \mathrm{tr}(\widetilde{g}_s \delta a^2 \widetilde{g}_s)$, this expression can also be written as $\sum_s \widetilde{p}_s \mathrm{tr}(\widetilde{g}_s \delta a^2 \widetilde{g}_s)$, so that the traces are all non-negative numbers.

From (5.28) and (5.29) it follows that the commutator of δa and δb is $[\delta a, \delta b] = [a, b] = \mathrm{i}c$. Now we introduce a real variable λ and multiply the matrix $\delta a + \mathrm{i}\lambda\delta b$ with its hermitean conjugate $\delta a - \mathrm{i}\lambda\delta b$, and take the expectation value, obtaining

$$\langle (\delta a - \mathrm{i}\lambda\delta b)(\delta a + \mathrm{i}\lambda\delta b)\rangle = \Delta a^2 + \lambda^2 \Delta b^2 - \lambda\langle c\rangle. \tag{5.31}$$

But the left side of this equation can be written

$$\sum_s \widetilde{p}_s \mathrm{tr}(\widetilde{g}_s(\delta a + \mathrm{i}\lambda\delta b)(\delta a - \mathrm{i}\lambda\delta b)\widetilde{g}_s),$$

where $\widetilde{g}_s(\delta a + \mathrm{i}\lambda\delta b)$ is the hermitean conjugate of $(\delta a - \mathrm{i}\lambda\delta b)\widetilde{g}_s$, so that the traces are all non-negative numbers, and as the probabilities $\widetilde{p}_s$ are also non-negative, both sides of (5.31) are non-negative. To make the most of this result, we choose the value of λ which gives the right side its minimum value, i.e., $\lambda = \frac{1}{2}\langle c\rangle/\Delta b^2$. The minimum value is still non-negative, and we thus obtain the result $\Delta a^2 \geq \frac{1}{4}\langle c\rangle^2/\Delta b^2$, or

$$\Delta a \Delta b \geq \tfrac{1}{2} |\ \langle c\rangle\ | \,. \tag{5.32}$$

This is the general form of Heisenberg's relations, and shows that if $\langle c\rangle \neq 0$, the uncertainty in one of the observables a and b must increase as the uncertainty in the other decreases: it is impossible to predict the measured values of both observables exactly.

If we choose $b = \widehat{a}$, where

$$[a, \widehat{a}] = \pm\mathrm{i}\hbar, \tag{5.33}$$

then a and $\widehat{a}$ are complementary observables, and (5.32) reduces to the form already given in (1.27). In non-relativistic quantum mechanics, the cartesian components X_α of the centre of mass vector $\mathbf{X}$ of any system (defined as the ratio of central vector $\mathbf{C}$ to its mass M) and the corresponding components K_β of the momentum $\mathbf{K}$ satisfy the commutation relations $[X_\alpha, K_\beta] = \mathrm{i}\hbar\delta_{\alpha\beta}$, so that X_α and K_α are complementary observables in this sense.

5.4 Special Relativistic Quantum Mechanics

The earliest attempts to develop a special relativistic quantum mechanics were based on the relation (5.6), or

$$E^2/c^2 = \mathbf{k}^2 + m^2c^2 \tag{5.34}$$

for a particle of momentum $\mathbf{k}$ and mass m free of external interactions. From classical electrodynamics, it was known that the energy E of a particle with electric charge e in interaction with an electromagnetic field should be regarded as including a term $e\varphi$, where φ is the scalar potential of the field, and that the momentum $\mathbf{k}$ should similarly be regarded as including a term $e\mathbf{A}/c$, where $\mathbf{A}$ is the vector potential of the field, obtained as in (4.28) from the solution of Maxwell's equations. On this basis it was concluded that the appropriate modification of (5.34) for a charged particle was

$$(E - e\varphi)^2/c^2 = (\mathbf{k} - e\mathbf{A}/c)^2 + m^2c^2. \tag{5.35}$$

The first attempts to explain the fine structure of the spectrum of the hydrogen atom were in fact based on the above equation. By substituting $\varphi = -e/(4\pi r)$ and $\mathbf{A} = 0$, the equation

$$E^2/c^2 - m^2c^2 = \mathbf{k}^2 - 2\alpha\hbar E/(cr) - \alpha^2\hbar^2/r^2$$

$$= k_r^2 + [l(l+1) - \alpha^2]\hbar^2/r^2 - 2\alpha\hbar E/(cr) \qquad [\alpha = e^2/(4\pi\hbar c)] \tag{5.36}$$

was obtained, which may be compared with the corresponding non-relativistic equation (5.18). The equations are of similar type, and their approximate equivalence can be verified by substituting $E = mc^2 + B$, where B is very small compared with mc^2. The eigenvalues B_ν of B are now given by

$$(2m + B_\nu/c^2)B_\nu = -\alpha_\nu^2, \qquad \alpha_\nu\beta_\nu = (m + B_\nu/c^2)Ze^2,$$

$$\beta_\nu = (\lambda + \nu)\hbar, \qquad \lambda(\lambda+1) = l(l+1) - \alpha^2, \tag{5.37}$$

instead of (5.20).

The most significant new feature in (5.37) is the appearance of the fine structure constant $\alpha \simeq 1/137.036$, and even this is quite small. Nevertheless, spectroscopic measurements were of such accuracy that it was recognized that the result of (5.34) could not be correct for the hydrogen atom, and it was only more recently that applications were found for bound states of two particles of spin zero, such as pionium, the short-lived bound state of positively and negatively charged π-mesons.

To obtain a correct account of the fine structure of the hydrogen atom it was necessary to take account of the spin of the electron, and this can done in a satisfactory way by the use of Dirac's equation instead of (5.34). Dirac observed that (5.34) can be converted to a linear equation by taking a matrix square root of the right side, thus:

$$E/c = \gamma_0(\boldsymbol{\gamma}\cdot\mathbf{k} + mc) \tag{5.38}$$

where the matrices γ_1, γ_2 and γ_3 forming the cartesian vector $\boldsymbol{\gamma}$, together with γ_0, must satisfy the relations (3.30), including

$$\gamma_\lambda\gamma_\mu + \gamma_\mu\gamma_\lambda = 2g_{\lambda\mu},$$

so that $\gamma_0^2 = (\gamma_\alpha\gamma_0)^2 = 1$. To take account of interactions with the electromagnetic field, as usual we replace E by the kinetic energy $E - e\varphi$ and $\mathbf{k}$ by the kinetic momentum $\mathbf{k} - e\mathbf{A}/c$ in (5.38), obtaining

$$E - e\varphi - c\gamma_0[\boldsymbol{\gamma}\cdot(\mathbf{k} - e\mathbf{A}/c) + mc] = 0. \tag{5.39}$$

Because φ and $\mathbf{A}$ do not commute with $\mathbf{k}$, the above equation is not exactly equivalent to (5.35). Indeed, if we multiply on the right by

$$E - e\varphi + c\gamma_0[\boldsymbol{\gamma}\cdot(\mathbf{k} - e\mathbf{A}/c) + mc],$$

we obtain

$$(E - e\varphi)^2/c^2 = (\mathbf{k} - e\mathbf{A}/c)^2 + m^2c^2 + [e\varphi, c\gamma_0\boldsymbol{\gamma}\cdot\mathbf{k}], \tag{5.40}$$

with an additional term which makes a small but significant contribution to the energy.

To determine the energy levels of the hydrogen atom, we again set $\varphi = -e/(4\pi r)$ and $\mathbf{A} = 0$, obtaining

$$E^2/c^2 - m^2c^2 = k_r^2 + (\mathbf{l}^2 - \alpha^2\hbar^2)/r^2 - 2\alpha\hbar E/(cr) + \mathrm{i}\alpha\hbar^2\gamma_0\boldsymbol{\gamma}\cdot\mathbf{r}/r^3. \tag{5.41}$$

instead of (5.36). Moreover, $\mathbf{l}^2$ does not commute with $\boldsymbol{\gamma}\cdot\mathbf{r}$, and so may not be replaced by its eigenvalue $l(l+1)\hbar^2$. We therefore introduce the total angular momentum,

$$\mathbf{j} = \mathbf{l} + \mathbf{s}, \qquad \mathbf{s} = \tfrac{1}{2}\hbar\gamma_0\gamma\gamma_4 \tag{5.42}$$

including the spin angular momentum $\mathbf{s}$ which has cartesian components $s_\alpha = \frac{1}{2}\hbar\sigma_\alpha = \frac{1}{2}\hbar\gamma_0\gamma_\alpha\gamma_4$, according to (3.21). The invariant $\mathbf{j}^2$ of $so(3)$ now commutes with $\boldsymbol{\gamma}\cdot\mathbf{r}$, and $\mathbf{s}^2 = \frac{3}{4}\hbar^2$, so that

$$\mathbf{l}^2 = \mathbf{j}^2 - 2\mathbf{l}\cdot\mathbf{s} - \mathbf{s}^2 = (j+\tfrac{1}{2})^2\hbar^2 - 2\mathbf{l}\cdot\mathbf{s} - \hbar^2,$$

where j, the maximum eigenvalue of j_3, is a half-integer $l \pm \frac{1}{2}$. When this result is substituted into (5.41), we have

$$E^2/c^2 - m^2c^2 = k_r^2 + [(j+\tfrac{1}{2})^2 - \alpha^2]\hbar^2/r^2 - 2\alpha\hbar E/(cr) + \kappa\hbar^2/r^2,$$

$$\kappa = -(2\mathbf{l}\cdot\mathbf{s}/\hbar^2 + 1) + \mathrm{i}\alpha\mathbf{r}\cdot\mathbf{s}\gamma_4/r \tag{5.43}$$

If the eigenvalue of $\mathbf{l}^2$ is $(j - \frac{1}{2})(j + \frac{1}{2})\hbar^2$, the eigenvalue of $2\mathbf{l}\cdot\mathbf{s}/\hbar^2 + 1$ is $(j + \frac{1}{2})$, and if the eigenvalue of $\mathbf{l}^2$ is $(j + \frac{1}{2})(j + \frac{3}{2})\hbar^2$, the eigenvalue of $2\mathbf{l}\cdot\mathbf{s}/\hbar^2 + 1$ is $-(j + \frac{1}{2})$, so that

$$(2\mathbf{l}\cdot\mathbf{s}/\hbar^2+1)^2=(j+\tfrac{1}{2})^2.$$

Also, by using $\mathbf{l}\cdot\mathbf{r}=0$ and the commutation rules $[l_\alpha,r_\beta]=\mathrm{i}\hbar\sum_\gamma\epsilon_{\alpha\beta\gamma}r_\gamma$, *or* by noticing that $\mathbf{r}\cdot\mathbf{s}$ does not commute with $2\mathbf{l}\cdot\mathbf{s}/\hbar^2+1$ and must therefore change the sign of its eigenvalue, we obtain

$$(2\mathbf{l}\cdot\mathbf{s}/\hbar^2+1)\mathbf{r}\cdot\mathbf{s}+\mathbf{r}\cdot\mathbf{s}(2\mathbf{l}\cdot\mathbf{s}/\hbar^2+1)=0.$$

Thus it follows from (5.41) and (5.42) that

$$E^2/c^2-m^2c^2=k_r^2+[\kappa(\kappa+1)-\alpha^2]\hbar^2/r^2-2\alpha\hbar E/(cr),$$

$$\kappa^2=(j+\tfrac{1}{2})^2-\alpha^2. \tag{5.44}$$

A comparison with (5.36) shows that the effect of the spin of the electron on the energy levels is to replace l with κ, which has *two* eigenvalues with opposite signs, and depends on the fine structure constant. The fine structure of the energy levels derived from (5.44) is in very good agreement with the spectroscopic data; nevertheless very precise measurements by Lamb and others revealed minute discrepancies which were only resolved following the development of a relativistic quantum electrodynamics.

5.4.1 Elastic Scattering

The calculation of cross-sections for scattering, within the special theory of relativity, is best done using the techniques of quantized field theory, which will be developed in the next chapter. Here we shall therefore discuss briefly only the relativistic kinematics of two particles which initially approach one another from a distance, are elastically scattered by their mutual interaction, and separate so as to finally recede from one another. It is a consequence of the uncertainty relations (5.32) that in a finite region of the real world the momenta of the particles cannot be known exactly, but in a sufficiently large region the uncertainty may be neglected, and in most scattering calculation it is assumed that precise information is available concerning the momenta $\mathbf{k}^{(1)}$ and $\mathbf{k}^{(2)}$ of the particles in the initial state. As shown in (5.15), if the rest masses of the particles are $m^{(1)}$ and $m^{(2)}$, these momenta can be expressed in terms of the total momentum $\mathbf{K}=\mathbf{k}^{(1)}+\mathbf{k}^{(2)}$ and a relative momentum $\mathbf{k}=(m^{(2)}\mathbf{k}^{(1)}-m^{(1)}\mathbf{k}^{(2)})/M$, where $M=m^{(1)}+m^{(2)}$ is the total mass, thus:

$$\mathbf{k}^{(1)}=m^{(1)}\mathbf{K}/M-\mathbf{k},\qquad \mathbf{k}^{(2)}=m^{(2)}\mathbf{K}/M+\mathbf{k}.$$

By a Lorentz transformation, the total momentum $\mathbf{K}$ can be reduced to zero, in what is known as the *barycentric* (centre-of mass) inertial frame, so that the initial momenta are simply $-\mathbf{k}$ and $\mathbf{k}$. In the process of scattering, the total momentum remains unchanged, and the momenta of the particles after scattering may therefore be denoted by $-\mathbf{k}'$ and $\mathbf{k}'$. The total energy of the particles in the initial state in the special theory of relativity is

$$c(\mathbf{k}^{(1)2}+m^{(1)2}c^2)^{\frac{1}{2}}+c(\mathbf{k}^{(2)2}+m^{(2)2}c^2)^{\frac{1}{2}}$$

according to (5.34), and reduces to $c(\mathbf{k}^2+m^{(1)2}c^2)^{\frac{1}{2}}+c(\mathbf{k}^2+m^{(2)2}c^2)^{\frac{1}{2}}$ in the barycentric frame. As the total energy also remains unchanged in the process of scattering, it is clear that $\mathbf{k}'^2=\mathbf{k}^2$. The angle of scattering θ in the barycentric frame is therefore given by

$$\cos\theta=\mathbf{k}\cdot\mathbf{k}'/\mathbf{k}^2.$$

The quantum theory does not of course allow the angle θ to be predicted for a particular scattering process, but the probability that the direction of $\mathbf{k}'$ will be found to be in any small solid angle $d\Omega$ is given by the differential cross-section as shown in (5.25). Experimentally it is possible to measure tbe momentum $\mathbf{k}'$ of one of the particles in the barycentric frame with any desired accuracy and an independent measurement of the momentum of the other particle then yields the value $-\mathbf{k}'$. It has sometimes been stated that the correlation of independent measurements of this type implies some sort of action at a distance, but this is surely a mistake. What is true is that the accurate measurement of the momentum of any particle can be made only with apparatus extending over a large volume, so that the process of measurement is non-local; furthermore, when the momentum of one of two particles in the barycentric frame is measured, the momentum of the other becomes a selected observable and the unpredictability associated with many quantal measurements is reduced to zero. The distinction between selected and unselected observables will be discussed in some detail in the next section, and a general quantal theory of measurement will be presented in Sect. 8.1.

Most of the first relativistic calculations of differential cross-sections for scattering were made in the context of quantum electrodynamics. Formal expressions for the cross-sections were obtained as power series in the fine-structure constant α, as defined in (5.36); these expressions, when expressed in terms of the physical charge e and mass m of the electron, were free of the ultra-violet divergences which had beset earlier non-relativistic calculations, but the power series in α were still only semi-convergent. Still, very good agreement with experiment was found by summing the first few terms of the power series representing the differential cross-sections obtained for the three elastic scattering processes of quantum electrodynamics:

(i) Rutherford scattering, i.e., the scattering of one electron by another $(m^{(1)}=m^{(2)}=m)$;

(ii) Compton scattering, i.e., the scattering of a photon by an electron $(m^{(1)}=m,\ m^{(2)}=0)$;

(iii) the scattering of one photon by another $(m^{(1)}=m^{(2)}=0)$.

The leading term of the cross-section for the last process is proportional to α^2 and the probability that one photon will scatter another is extremely small, but there are experiments with atoms and lasers in which it can be detected.

Confidence in the validity of quantized field theory has increased since the extension of its successes to predicting the cross-sections for *electro-weak*

interactions, in which neutrinos as well as electrons are involved, as well as a variety of other observable quantities. It has had more limited success in modelling strong interactions with unified theories in which the elementary particles include *quarks* and *gluons*. One of the ideas motivating the development of string theory was the possibility of unifying the force of gravity with the electro-weak and strong interactions. We shall discuss these ideas in somewhat more detail in the next chapter.

5.5 Selected and Unselected Observables

An observable is represented by a matrix a which can be expressed in the form

$$a = \sum_r a_r g_r, \qquad g_r g_s = g_r \delta_{rs}, \qquad \sum_r g_r = 1, \qquad \mathrm{tr}(g_r) = 1. \tag{5.45}$$

As can be seen from (2.3), a qubit is an observable in this sense, but in general r takes N values, where N may be finite, countably infinite or uncountably infinite. The a_r are identified with the possible results of a measurement of the observable and although the g_r in (5.45) are matrices, their definition is fully compatible with the classical definition already given in (1.13) and (1.14). The condition $\mathrm{tr}(g_r) = 1$ implies that the g_r are *minimal* projections with only one non-vanishing eigenvalues 1. Where b is uncountably infinite, the summation $\sum_r$ is normally interpreted as an integration $\int dr$ over a continuous range of values of r, and the *spectrum* of the corresponding eigenvalues a_r of a is also continuous; but it is possible for r to take a finite or countably infinite set of discrete values as well. If a is an observable of a system at rest in the inertial frame of the conscious observer, it is assumed to be hermitean.

One of the attributes of consciousness is the ability to gain information, and it would seem reasonable, therefore, to infer that information concerning an event is normally gained by a conscious observer. *After* the observation has been made, the outcome of the event is certain and information to be gained is reduced to zero. Here we shall recognize that the outcome of an event may be predictable, so that the observation merely confirms what could, in principle, be inferred from sufficient antecedent information derived from other sources. Then the information obtained from observation of the event will be called *selected*. The information derived from the observation of the outcome of most macroscopic events, such as an eclipse of the moon, is selected in this sense. Sometimes, as for the winning of a horse race, the prediction is possible only a very short time before the actual event. But we shall show later that there are other events, such as the decay of a radioactive atom within a given period of time, that are are completely unpredictable, and the information derived from the observation of such an event will be called unselected. The selected information concerning a particular system is encoded in a special observable

P, called the *statistical matrix*, following von Neumann's terminology; Dirac's *density matrix* has much the same significance.

To make the conditions for selection more precise, suppose that a is any observable, and that P is the statistical matrix. Then the probability that a measurement of a will yield the value a_r is

$$p_r = \mathrm{tr}(g_r P), \tag{5.46}$$

and the expectation value of a is

$$\langle a \rangle = \sum a_r p_r = \mathrm{tr}(aP). \tag{5.47}$$

The *quantal information* to be gained from the measurement is

$$I = \sum \log(p_r) g_r, \tag{5.48}$$

where the projections g_r are uniquely associated with the observable a. The expectation value of I is

$$\langle I \rangle = -\mathrm{tr}(IP) = -\sum \log(p_r) p_r. \tag{5.49}$$

This is the *classical information* to be gained, as defined by Shannon; it is a positive number that, unlike the quantal information I, gives no indication of what the information is about.

A *selected* observable is one that commutes with the statistical matrix. If $\tilde{a} = \sum \tilde{a}_s \tilde{g}_s$ is a selected observable, then

$$P = \sum \tilde{p}_s \tilde{g}_s. \tag{5.50}$$

On the other hand, the probability that a measurement will yield the eigenvalue a_r of the *unselected* observable a as defined in (5.45), obtained from (5.46) and (5.50), is

$$p_r = \sum p_{rs} \tilde{p}_s, \qquad p_{rs} = \mathrm{tr}(g_r \tilde{g}_s), \tag{5.51}$$

The p_{rs} satisfy

$$\sum_r p_{rs} = \sum_s p_{rs} = 1, \tag{5.52}$$

and reduce to δ_{rs} when a is the same as the selected observable $\tilde{a}$. Since $p_{rs} = \mathrm{tr}(g_r \tilde{g}_s g \tilde{g}_s g_r)$, where $\tilde{g}_s g_r$ is the hermitean conjugate of $g_r \tilde{g}_s$, it is always positive and may be interpreted as the *conditional probability* of observing the value a_r of a, *if* the value of the observable $\tilde{a}$ is $\tilde{a}_s$.

5.6 The Fundamental Observables of Physics

In this section our aim will be to give quantal definitions of the fundamental observables of a physical system, consistent with the definitions based on the Principle of Least Action in Sect. 1.2.

If a system occupies a definite region Ω of space and time it is easily distinguished from its environment. If there are external gravitational and electromagnetic interactions they can be approximated by their expectation values, which are those of classical physics. The energy is usually assumed to include the energy of interaction with external fields, and there may also be contributions from external sources to other fundamental observables. Nevertheless, in (1.9) we have have given valid definitions of the fundamental observables: the energy E, the momentum $\mathbf{K}$, the angular momentum $\mathbf{J}$ and the central vector $\mathbf{C}$, and the 'charges' Q_1, Q_2, ... of a physical system in terms of the action A. The action A was identified as the fundamental additive observable used to specify the state of the system, depending only on a set of parameters (x) which constitute the frame of reference.

In quantum mechanics, on the other hand, the state of a system S is represented by the statistical matrix P, and it follows that the action in any inertial frame should determine and be determined by P when expressed in the *Schrödinger representation, i.e.*, in terms of the set of parameters $(x) = (t, \mathbf{x}, \mathbf{u}, \mathbf{v}, \xi^1, \xi^2, ...)$ which specify the frame. For the present purpose we shall therefore regard P as a function $P(x)$ or $P(t, \mathbf{x}, \mathbf{u}, \mathbf{v}, \xi^1, \xi^2, ...)$ of the time t, position $\mathbf{x}$, orientation $\mathbf{u}$ and velocity $\mathbf{v}$ of the observer. In any inertial frame, the eigenvalues of P are the probabilities $\widetilde{p}_r$ that the measurement of any selected observable O will yield the value $\widetilde{o}_r$ and must be same for all observers, and as $P(x)$ is hermitean it must be related to its value $P(0)$ in the inertial frame of an observer at the origin by a unitary transformation:

$$P(x) = U(x)P(0)U^\dagger(x) \tag{5.53}$$

where $U = U(x)$ satisfies the unitary condition $U^\dagger = U^{-1}$.

Let us now consider a system S consisting of two or more sub-systems $\mathrm{S}^{(1)}$, $\mathrm{S}^{(2)}$, ... in a region Ω of space-time, which are not in interaction and have not interacted previously, so that they are statistically independent of one another. Since the joint probability of two independent events is the product of the probabilities of the separate events, the statistical matrix P of the composite system is then the direct product $P^{[1]} \otimes P^{[2]}...$ of the statistical matrices $P^{[1]}$, $P^{[2]}$, ... of the sub-systems; we can therefore write $P = P^{(1)}P^{(2)}...$ where $P^{(1)} = P^{[1]} \otimes 1...$, $P^{(2)} = 1 \otimes P^{[2]}....$ Moreover, if $P^{[1]}(x) = U^{[1]}(x)P^{[1]}(0)U^{[1]\dagger}(x)$, $P^{[2]}(x) = U^{[2]}(x)P^{[2]}(0)U^{[2]\dagger}(x)$, ...then

$$U(x) = U^{(1)}(x)U^{(2)}(x)..., \tag{5.54}$$

where $U^{(1)} = U^{[1]} \otimes 1...$, $U^{(2)} = 1 \otimes U^{[2]}....$ Thus in the quantum theory

$$A(x) = \mathrm{i} \log U(x) = \mathrm{i}(\log U^{(1)} + \log U^{(2)} + ...) \tag{5.55}$$

is an invariant observable defined on a region of space-time which is additive for non-interacting systems and, in suitable units, *may be identified with the action*. The imaginary unit is required because A is an observable, and therefore hermitean, while U is unitary. Thus

$$U(x) = \exp[-\mathrm{i}A(x)/\hbar] \tag{5.56}$$

where $\hbar$ is the universal unit of action as defined in (1.27). Also, for a small change (δx) of the parameters (x), the change in $U(x)$ is

$$\delta U(x) = -\mathrm{i}\delta A(x)U(x)/\hbar,$$

$$\delta A(x) = E\delta t - \mathbf{K} \cdot \delta d\mathbf{x} - \mathbf{J} \cdot \delta \mathbf{u} + \mathbf{C} \cdot \delta \mathbf{v} + Q_1 \delta \xi^1 + Q_2 \delta \xi^2 + ..., \tag{5.57}$$

This is regarded as the *quantal* definition of the energy E, the momentum $\mathbf{K}$, the angular momentum $\mathbf{J}$, the central vector $\mathbf{C}$ and the 'charges' Q_1, Q_2, ... of the system, and is clearly equivalent to the classical definition given in Sect. 1.2.

5.6.1 Schrödinger's Wave Mechanics

We have already seen in the introduction to this chapter that in quantum mechanics the fundamental observables E, $\mathbf{K}$, $\mathbf{J}$, and $\mathbf{C}$ in (5.57) do not all commute with one another, and even different components of the same vector (such as the components J_1, J_2 and J_3 of $\mathbf{J}$) do not commute. This can be regarded as a consequence of the fact that all the observables depend on the parameters of the inertial system (x) relative to the fixed inertial system (0). Nevertheless, the result of (5.57) shows that the unitary matrix $U = U(x)$ satisfies the partial differential equations

$$\mathrm{i}\hbar \frac{\partial U}{\partial t} = EU, \qquad -\mathrm{i}\hbar \frac{\partial U}{\partial \mathbf{x}} = \mathbf{K}U,$$

$$-\mathrm{i}\hbar \frac{\partial U}{\partial \mathbf{u}} = \mathbf{J}U, \qquad \mathrm{i}\hbar \frac{\partial U}{\partial \mathbf{v}} = \mathbf{C}U. \tag{5.58}$$

The first two of these equations were postulated by Schrödinger as the basis of his wave mechanics, except that he assumed that the microscopic system could be represented by a single wave function $\Psi(t, \mathbf{x})$, depending simply on the time t and the position $\mathbf{x}$ when the orientation $\mathbf{u}$ and the velocity $\mathbf{v}$ of the observer had fixed values. The present derivation shows that Schrödinger's wave function should be regarded as an element of the unitary matrix U. The conditions under which the state of a physical system can be represented by a single wave function are quite exceptional: they are retrospective, and assume that ideal measurements have been made and imply that as a result of

these measurements the information concerning the system is effectively complete. Schrödinger was an idealist and was never able to accept the statistical interpretation of quantum mechanics.

From (5.52) and (5.58) we have

$$\mathrm{i}\hbar\frac{\partial P}{\partial t} = HP - PH, \qquad -\mathrm{i}\hbar\frac{\partial P}{\partial \mathbf{x}} = \mathbf{K}P - P\mathbf{K},$$

$$-\mathrm{i}\hbar\frac{\partial P}{\partial \mathbf{u}} = \mathbf{J}P - P\mathbf{J}, \qquad \mathrm{i}\hbar\frac{\partial P}{\partial \mathbf{v}} = \mathbf{C}P - P\mathbf{C}. \tag{5.59}$$

In the absence of external interactions causing variations in the energy, a system may be in what is known as a *stationary* state not depending on the time, so that $HP = PH$, and the energy is what we have called a selected observable. Similarly, in the absence of external interactions causing variations in the momentum, $\mathbf{K}P = P\mathbf{K}$, and the momentum is a selected observable. Under special conditions, the angular momentum $\mathbf{J}$ or the central vector $\mathbf{C}$ may also be selected observables.

5.6.2 The Heisenberg Representation

The Schrödinger representation is one of three in common use in quantum mechanics; the original formulation in terms of matrices was in what is known as the *Heisenberg* representation, which is also used extensively in quantized field theories. It is therefore important to make a distinction between an observable O in the Heisenberg representation and the corresponding observable O^{S} in the Schrödinger representation. In the Schrödinger representation, it is the statistical matrix that depends on the inertial frame, but observables, like E, $\mathbf{K}$, $\mathbf{J}$, and $\mathbf{C}$ in (5.58), are independent of the frame. On the other hand, in the Heisenberg representation, the statistical matrix $P = P(0)$ is always the same and can be identified with that of a fixed observational system at the origin of coordinates, but it is the observables that depend on the frame of reference of the observer in which any measurement is made. But the expectation value of an observable is independent of the representation, and

$$\langle O\rangle = \langle O^{\mathrm{S}}\rangle = \mathrm{tr}[O^{\mathrm{S}}P(x)],$$

in terms of the statistical matrix $P(x)$ of the Schrödinger representation. However, in the Heisenberg representation we rewrite (5.53) as $P(x) = U(x)PU^{\dagger}(x)$, so that the expectation value becomes

$$\langle O\rangle = \mathrm{tr}[U^{\dagger}(x)O^{\mathrm{S}}U(x)P] = \mathrm{tr}[O(x)P(0)], \qquad O(x) = U^{\dagger}(x)O^{\mathrm{S}}U(x), \tag{5.60}$$

and the observable $O = O(x)$ is now a functions of the parameters (x) of the inertial frame in which it is measured. A similar transformation can be made of all other observables, including the total energy, momentum and angular momentum.

It follows from (5.58 and (5.60) that, in the Heisenberg representation any observable depends on the frame of reference of the observer in accordance with the fundamental relations

$$\mathrm{i}\hbar\frac{\partial O}{\partial t} = OE - EO, \qquad -\mathrm{i}\hbar\frac{\partial U}{\partial \mathbf{x}} = O\mathbf{K} - \mathbf{K}O,$$

$$-\mathrm{i}\hbar\frac{\partial O}{\partial \mathbf{u}} = O\mathbf{J} - \mathbf{J}O, \qquad \mathrm{i}\hbar\frac{\partial O}{\partial \mathbf{v}} = O\mathbf{C} - \mathbf{C}O. \tag{5.61}$$

5.6.3 The Interaction Representation

A third representation is commonly used in the consideration of a system S consisting of a set of sub-systems $\mathrm{S}^{(p)}$ $(p = 1, 2, ...)$ in interaction. The total energy E at time t, in the inertial frame of an observer at the origin in space, is then a sum of the energies $E^{(p)}$ of the sub-systems, together with an interaction energy V depending on the observables of the sub-systems. In most applications, it is assumed that the statistical matrix P of S is known in terms of the corresponding matrices $P^{(p)}$ of the $\mathrm{S}^{(p)}$ at some initial time $t = t_i$, usually because the sub-systems have not been in interaction previously, or because their correlations are negligible for other reasons, so that the initial value P_i of P can be expressed as the direct product $P_i = P_i^{(1)}P_i^{(2)}\dots$. The use of the *interaction representation* is a method for the study of the interactions of such a composite system; it has its uses in quantized field theory, but also has many other applications. The principal object is to construct a time-dependent unitary matrix T connecting any observable O with the corresponding observable O_0 in the absence of interaction. It is unnecessary to consider the variation of the unitary matrix U of (5.58) with the parameters (x) of the frame of reference other than the time, so that

$$i\hbar\frac{dU}{dt} = EU = (E_0 + V)U, \qquad E_0 = \sum_p E^{(p)}. \tag{5.62}$$

The T-matrix and its hermitean conjugate $T^{\dagger}$ are required to satisfy the equations

$$\mathrm{i}\hbar\frac{dT}{dt} = TV, \qquad \mathrm{i}\hbar\frac{dT^{\dagger}}{dt} = -VT^{\dagger}, \tag{5.63}$$

and have the value 1 at time t_i. Then it follows from (5.63) that $T^{\dagger}T$ has the constant value 1, and T is unitary, as required. In the interaction representation any observable $\tilde{O}$ is defined by

$$\tilde{O} = TOT^{\dagger}, \tag{5.64}$$

so that, as a consequence of (5.61) and (5.63),

$$i\hbar\frac{d\tilde{O}}{dt} = T(i\hbar\frac{dO}{dt} - [O,V])T^\dagger = T[O,E_0]T^\top = [\tilde{O},\tilde{E}_0]. \tag{5.65}$$

If E_0 is expressed in terms of other observables, $\tilde{E}_0$ is expressed in terms of the same observables in the interaction representation. Also, $TV = \tilde{V}T$ and as $T = 1$ at the initial time t_i, it follows from (5.63) that T also satisfies the integral equation

$$T(t) = 1 - i\int_{t_i}^{t} \tilde{V}(t_1)T(t_1)dt_1/\hbar. \tag{5.66}$$

This equation can be solved by iteration, i.e., repeated substitution from the left into the right side, yielding

$$T(t) = 1 - i\int_{t_i}^{t} \tilde{V}(t_1)dt_1/\hbar - \int_{t_i}^{t} \tilde{V}(t_1)dt_1 \int_{t_i}^{t_1} \tilde{V}(t_2)dt_2/\hbar^2 + ...$$

This is the result of perturbation theory, but as the infinite series is at best semi-convergent when t is large, other methods are preferable and have been developed.

Again the expectation value $\langle O\rangle = \mathrm{tr}(OP)$ of an observable O at time t must be independent of the representation; in the Heisenberg representation P is independent of the time, though O in general depends on the time. However, it follows from (5.65) that

$$\langle O\rangle = \mathrm{tr}(OP) = \mathrm{tr}(\tilde{O}\tilde{P}), \qquad \tilde{P} = TPT^\dagger, \tag{5.67}$$

where $\tilde{P}$ is now the statistical matrix in the interaction representation, and like O depends on the time though in the absence of interactions there is no difference between P and $\tilde{P}$.

5.7 Statistical Physics

In the study of systems consisting of a small number of particles it has been usual, from the time of Newton and even up to the present day, to assume that a maximum of information, within the constraints imposed by the Uncertainty Principle, is available concerning the system. On the other hand, macroscopic systems normally consist of extremely large numbers of particles concerning which very little information is available, and for the quantitative description of these it has been necessary to develop statistical methods very different from those of particle physics. The origins of statistical physics can be traced to the work of Boltzmann and Maxwell in formulating the kinetic theory of gases. To Boltzmann we owe the idea that the *entropy* associated with a particular state of a system, as defined in the context of thermodynamics by Clausius, should be identified as $-\log p_r$, where p_r is the probability of finding the system in that state. In the light of Shannon's definition

of information, this implied the equivalence of entropy with information to be gained. The general concepts of statistical mechanics were developed by Gibbs, following important contributions by Liouville, near the end of the nineteenth century. During the twentieth century much progress has been made in applications to the statistical thermodynamics and irreversible statistical mechanics of solids and liquids. In Chap. 8 we shall discuss the application to electrolytes, but for the present we shall be concerned only with general principles.

For a system in equilibrium with its environment, the selected observables include the energy E, some combination of the momentum $\mathbf{K}$ and the angular momentum $\mathbf{L}$, and the numbers N_a of the different indivisible electrochemical constituents. To these we may add a numerical multiple W of the unit matrix, identified as the work function, and expressible as an integral $\int p d^3x$ of the pressure p over the volume of the region occupied by the system. The information to be gained from the measurement of these observables is $I = -\log P$, where P is as usual the statistical matrix. For a system consisting of a number of sub-systems in mechanical and thermodynamical equilibrium, it may be assumed, as in the argument leading from (5.53) to (5.54), that P is a product $P^{(1)}P^{(2)}...$ of the density matrices for the subsystems, so that $I = -\log P^{(1)} - \log P^{(2)} - ....$ The information to be gained, like the selected observables, is thus an additive function on the region V, and depends linearly on them:

$$I = \beta(E + W - \mathbf{u}\cdot\mathbf{K} - \boldsymbol{\omega}\cdot\mathbf{L} - \sum_a \chi_a N_a). \tag{5.68}$$

In agreement with Shannon's theory, the classical information $\langle I\rangle$ to be gained concerning the selected observables is the entropy S in appropriate units:

$$S = \beta\langle E + W - \mathbf{u}\cdot\mathbf{K} - \boldsymbol{\omega}\cdot\mathbf{L} - \sum_a \chi_a N_a\rangle. \tag{5.69}$$

This expression can only depend on the macroscopic quantities β, $\mathbf{u}$, $\boldsymbol{\omega}$ and the χ_a appearing in this relation, which by arguments essentially due to Gibbs are identified respectively as the inverse temperature, the translational and angular velocities, and potentials (with chemical, centrifugal, gravitational and electrical contributions in general).

At this point we shall simplify matters by assuming that $\mathbf{u}$ and $\boldsymbol{\omega}$ are both zero. Then

$$I = \beta\sum_r (E_r + W - \sum_a \chi_a N_{ar})g_r, \tag{5.70}$$

where the E_r and N_{ar} are simultaneous eigenvalues of E and N_a and the g_r are corresponding projections. Since the fundamental observables are selected, the statistical matrix P and the infomational observable I are directly connected by the relation $P = \exp(-I)$, and the former is given by

$$P = \exp[-\beta(E + W - \sum_{\alpha} \chi_a N_a)] = \sum_r \exp[-\beta(E_r + W - \sum_a \chi_a N_{ar})] g_r. \tag{5.71}$$

Since $\mathrm{tr}(P) = 1$, we obtain the well-known formula

$$\mathrm{e}^{\beta W} = \mathrm{tr}\{\exp[-\beta(E - \sum_{\alpha} \chi_a N_a)]\} = \sum_r \exp[-\beta(E_r - \sum_a \chi_a N_{ar})] \tag{5.72}$$

for the work function.

The inverse temperature β is defined more precisely as $1/(kT)$, where $k = 1.3806610^{-16}$ erg/deg K is Boltzmann's constant and T is the *absolute temperature*. In the states of thermodynmical equilibribrium of any system, β and the potentials χ_a have values independent of position and time. However, in information theory (5.68) serves to define the absolute temperature and potentials, and the relations derived from it are identities. The latter are therefore also valid for a subsystem occupying any region which is sufficiently small for variations in β and the χ_a to be neglected, even within a system which is not in a state of thermodynamic equilibrium. *In such a state of an extended system, the temperature and potentials may vary with position and time.*

The quantum mechanics of systems with large numbers of interacting particles poses difficult computational problems in general. Exact solutions for a variety of two-dimensional lattice problems have been obtained by the free fermion method or *via* the Yang-Baxter equation; these can be given a formulation in which elements of the underlying Lie algebras are represented by fermions or parafermions, and thus in terms of qubits. But for disordered systems the known exact solutions are more limited. For bound states, with interactions which are quadratic functions of the coordinates, an exact analysis is possible in terms of harmonic oscillations or bosons. McGuire provided the first exact solution to the many-particle scattering problem, with delta-function interactions. Because of their mathematical complexity, we shall not discuss these often beautiful results further in the present volume.

5.7.1 Macroscopic and Microscopic Variables

Before the advent of quantum mechanics, and indeed before any clear understanding of the atomic structure of matter had beeen reached, macroscopic theories of solids and fluids were developed on the basis of Newtonian mechanics which were very successful in accounting for a variety of observed phenomena. Solids and fluids were both represented as indefinitely divisible media with densities of mass, momentum and energy which remained continuous and smooth at any level of magnification. One of the important features of statistical mechanics is that it can explain the successes of these theories and justify their use, in spite of their failure to take into acccount the actual microscopic structure, including the sub-microscopic structure of

matter. This is done by identifying various macroscopic quantities as *expectation values* of the corresponding microscopic quantitities. These macroscopic quantities include the fundamental observables of a system and their densities, and potentials and intensities of fields such as an electromagnetic field.

If A is a fundamental observable of any system, and therefore unchanged except by external interactions, it follows from (5.59) that at time t and at the point $\mathbf{x}$ of space

$$\mathrm{i}\hbar \frac{\partial(AP)}{\partial t} = E(AP) - (AP)E, \qquad -\mathrm{i}\hbar \frac{\partial(AP)}{\partial \mathbf{x}} = \mathbf{K}(AP) - (AP)\mathbf{K}. \tag{5.73}$$

The microscopic density associated with A is defined as

$$\rho_{A\mathrm{mic}} = \tfrac{1}{2}[(A\delta(\mathbf{x} - \mathbf{X}) + \delta(\mathbf{x} - \mathbf{X})A], \tag{5.74}$$

where $\mathbf{X} = \mathbf{C}/M$ is the centre-of-mass observable of the system obtained from the central vector $\mathbf{C}$ given by (5.58), and $\delta(\mathbf{x} - \mathbf{X})$ is a three-dimensional analogue of Dirac's delta-function appearing in (A.59). The essential property of this distribution is that if $\mathbf{X}_r$ is an eigenvalue of $\mathbf{X}$, then $\delta(\mathbf{x} - \mathbf{X}_r) = 0$ when $\mathbf{x} - \mathbf{X}_r \neq 0$ but

$$\int \delta(\mathbf{x} - \mathbf{X}_r) d^3x = 1.$$

The macroscopic density associated with A at the point $\mathbf{x}$ is then the expectation value

$$\rho_A = \langle \rho_{A\mathrm{mic}} \rangle = \mathrm{tr}[(AP\delta(\mathbf{x} - \mathbf{X})]. \tag{5.75}$$

The velocity of the system is $\mathbf{K}/M$ and the corresponding macroscopic *flux density* is therefore defined by

$$\boldsymbol{\sigma}_A = \mathrm{tr}[\tfrac{1}{2}(\mathbf{K}AP + AP\mathbf{K})/M]. \tag{5.76}$$

With the help of (5.7) it then follows from (5.71) and (5.75) that

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \boldsymbol{\sigma}_A = 0, \tag{5.77}$$

which is the *macroscopic conservation equation* for the observable A, and of the type which was the basis of much of the classical physics in which matter was assumed to be indefinitely divisible .

A simple but important application identifies A with the number of particles N_a of type a in the region which defines the system. Then ρ_A is the number density of particles of that type, usually denoted by n_a, and $\boldsymbol{\sigma}_A$ is the flux density, usually denoted by $n_a\mathbf{u}_a$ to define the *diffusion velocity* $\mathbf{u}_a$. The macroscopic conservation equation is then

$$\frac{\partial n_a}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (n_a \mathbf{u}_a) = 0. \tag{5.78}$$

As its derivation makes clear, the validity of this equation is not restricted to systems in thermodynamic equilibrium, and it is fundamental to theories of ordinary and thermal diffusion where the inverse temperature β and the potentials χ_a vary with position and time. In theories of irreversible processes, the flux densities $n_a \mathbf{u}_a$ are expressed linearly in terms of the gradients $\nabla\beta$ and $\nabla\chi_a$, thus:

$$n_a \mathbf{u}_a = \lambda_a \nabla\beta/\beta - \sum_b \lambda_{ab} \nabla\chi_b, \tag{5.79}$$

when these gradients are sufficiently small. The factors λ_a and λ_{ab} are coefficients of thermal and ordinary diffusion, and depend on the number densities n_a in general. A quantal derivation of *constitutive equations* of this type, based on the evaluation of the statistical matrix for non-equilibrium states, is due to Kubo, and has the merit that the coefficients of diffusion can be calculated in principle from a knowledge of the microscopic consitiution of the macroscopic system. Again the calculations are not simple and they will not be reproduced here, but we notice that, together with (5.78), constitutive equations such as (5.79) form the basis of various macroscopic theories of irreversible processes.

As an application of these ideas which will be needed in Sect. 8.2 we shall discuss the theory of electrolytes.

5.8 Theory of Electrolytes

The theory of electrolytes provides a relatively simple application of statistical physics. The particles are ions of various kinds which carry electric charge, but in an aqueous environment where the water molecules are strongly polarized and form an approximately spherical shell of hydration around any charge, so that the resultant electrical potential of the ion and its hydration shell decreases much more rapidly with distance from the ion than Coulomb's law would suggest.

In (5.78) we obtained what may in this context be interpreted as the equations of conservation of the various types of ions, connecting the ionic number densities n_a with the corresponding diffusion velocities $\mathbf{u}_a$. If e_a is the electric charge carried by an ion of the a-th type, the charge density ϵ_a and the current density $\mathbf{j}_a$ associated with ions of that type are

$$\epsilon_a = e_a n_a, \qquad \mathbf{j}_a = e_a n_a \mathbf{u}_a, \tag{5.80}$$

and, as a consequence of (5.78) satisfy the conservation equation

$$\frac{\partial \epsilon_a}{\partial t} + \nabla \cdot \mathbf{j}_a = 0. \tag{5.81}$$

The resultant charge density ϵ and current density $\mathbf{j}$ are obtained by summation over a:

$$\epsilon = \sum_\alpha \epsilon_a = \sum_a e_a n_a, \qquad \mathbf{j} = \sum_a \mathbf{j}_a == \sum_a e_a n_a \mathbf{u}_a, \tag{5.82}$$

and satisfy a similar conservation equation.

The ionic currents $\mathbf{j}_a$ are determined from a generalized form of Ohm's law implicit in (5.79), a constitutive equation which as we have seen may be based on an application of the theory of the statistical matrix to irreversible processes. In this application some justifiable approximations are required. Thermal diffusion is a minor effect and the coeffcient λ_a in (5.79) will be neglected; also, in an electrolyte where the ionic concentrations are not too large the ions are shielded from one another by the polarization of the water molecules of hydration and their interactions may be neglected, so that the coeffcients λ_{ab} with $b \neq a$ will also be neglected. Thus, when (5.79) is substituted into (5.80), we obtain the simple formula

$$\mathbf{j}_a = -e_a \lambda_a \nabla\chi_a = -\sigma_a \nabla(\varphi - \varphi_a), \qquad \sigma_a = e_a^2 \lambda_a, \tag{5.83}$$

for the ionic current density $\mathbf{j}_a$ in terms of the gradient $\nabla\chi_a$ or in terms of $\nabla(\varphi - \varphi_a)$, if.the electrochemical potentials are expressed in the form

$$\chi_a = e_a(\varphi - \varphi_a), \qquad e_a \varphi_\alpha = -m_a \mu_a. \tag{5.84}$$

Here φ is as usual the electrical potential, m_a is the the effective mass of an ion of the a-th type and μ_a is the chemical potential per unit mass of such an ion as defined in the chemical literature. The use of φ_a, which is the negative of the chemical potential per unit charge, has the advantage that in thermodynamical equilibrium φ_a differs from the electrical potential only by a constant. A general relation between the electrostatic potential and the charge density is provided by Coulomb's law of electrostatics. In an electrolyte of dielectric constant κ, the potential at the point $\mathbf{x}$ due to a hydrated electric charge e_a at the point $\mathbf{x} - \mathbf{r}$ is $e_a/(\kappa r)$, and it follows that the expectation value $(\varphi)$of the potential at the point $\mathbf{x}$ is given by

$$\nabla^2 \varphi = -(4\pi/\kappa) \sum_a \epsilon_a = -(4\pi/\kappa) \sum_a e_a n_a, \tag{5.85}$$

To determine the potentials φ and φ_a, the only other result required is an expression for the densities n_a in terms of the φ_a. In general the relation of the densities to the potentials requires the evaluation of the expression given in (5.72) for the work function W. This is not easy in general, but again it is possible to make use of the fact that, in an electrolyte where the ionic concentrations are not too large, the ions are shielded from one another by the polarization of the water molecules of hydration and their interactions may be neglected. We consider a region of volume δV in an electrolyte containing the point $\mathbf{x}$, which is so small that it can contain at most one ion, assumed to be of the a-th type. The work function is simply $n_a \delta V$ and if $\mathbf{k}$ is the momentum of the hydrated ion, its energy E is $\mathbf{k}^2/2m_a + e_a\varphi$. Thus, in

this simple application (5.72) reduces in a serviceable approximation to the formula

$$\exp(-\beta n_a \delta V) = n_a c_a \exp(-\beta e_a \varphi_a),$$

where c_a is a constant depending on the entropy associated with the ion. Since δV is very small, we infer that if the density of the a-th ionic constituent is not too large,

$$n_a = n_a^0 \exp(\beta e_a \varphi_a), \qquad \epsilon_a = \epsilon_a^0 \exp(\beta e_a \varphi_a), \tag{5.86}$$

where n_a^0 and $\epsilon_a^0 = e_a n_a^0$ are constants. If these expressions for the number and charge densities are substituted into (5.85), the latter becomes a differential equation from which, with suitable boundary conditions, the potentials may be determined.

5.8.1 The Debye–Hückel Equation

In thermodynamical equilibrium, the ionic currents $\mathbf{j}_a$ are all zero, and the differences between the potentials φ_a and φ have the same values throughout the electolyte. It then follows from (5.82) and (5.86) that

$$\epsilon_a = e_a n_a' \exp(-\beta e_a \varphi), \tag{5.87}$$

where $n_a' = n_a^0 \exp(\beta e_a \chi_a)$ is also a constant in thermodynamical equilibrium. Under the same conditions, by a suitable choice of the constants n_a^0 in (5.86) we can interpret the n_a' as number densities at some point where the charge density and potential are both zero, so that

$$\sum_a e_a n_a' = 0. \tag{5.88}$$

By combining these results with (5.85), we obtain what is known as the *Debye–Hückel equation*

$$\nabla^2 \varphi = -4\pi \sum_a (e_a n_a^0/\kappa) \exp(-\beta e_a \varphi), \tag{5.89}$$

valid only for thermodynamical equilibrium. If we assume an absolute temperature of ~ 300 K, a charge $e_a = e_K = 4.80324 \times 10^{-10}$ esu, and a potential of 25 mV, $\beta e_a \varphi \approx 1$. So, if the potential is less than ~ 20 mV, the exponential function in (5.89) may be approximated by $1 - \beta e_a \varphi$ and the equation reduces to

$$\nabla^2 \varphi = a_D^{-2} \varphi, \qquad a_D^{-2} = (4\pi/\kappa) \sum_a e_a^2 n_a^0, \tag{5.90}$$

where a_D is called the Debye shielding length, and has a value that is typically somewhat less than 10 Å in the nervous system of animals.

The solution depends on the information available. Given only that there is an ion of the a-th type at distance r from the point $\mathbf{x}$,

$$\frac{1}{r}\frac{d^2}{dr^2}(r\varphi) = a_D^{-2}\varphi,$$

which has the solution

$$\varphi = (e_a/r) \exp(-r/a_D) \qquad (r \geq d) \tag{5.91}$$

that reduces to e_a/r for small r. However, this Debye–Hückel potential is good only for sufficiently large values of r, partly because the approximation leading from (5.89) to (5.90) is valid only when φ is sufficiently small, and more significantly because it ignores the finite size of the ion. It is therefore better to regard (5.91) as valid when r is not less than the ionic diameter d, and where necessary assume that φ has the constant value $(e_a/d) \exp(-d/a_D)$ for $r \leq d$. It is easily confirmed from (5.91) that the expected potential due to an ion in an electrolyte falls quite rapidly to zero at large distances; this result can be attributed to the tendency of an ion to attract other ions, including H^+ or OH^- ions, of opposite charge, so that the expected total charge within a sufficiently large sphere surrounding an ion is zero.

5.9 Summary

The early sections of this chapter have been devoted mainly to problems motivated by the formulation of a common description of the various types of elementary particles in terms of the information which they convey concerning distant events to the observer. A general account of the special theory of relativity is followed by a discussion of the application of informational principles to non-relativistic quantum mechanics and its associated uncertainty relations, then of special relativistic quantum mechanics in similar terms. Some emphasis is put on the distinction between selected observables the result of whose measurement is in principle predictable, and unselected observables concerning which no independent information is available and whose measured values are therefore quite unpredictable.

6. Quantized Field Theories

Although the concept of information was so slow to develop in classical physics, the more difficult concept of a field of force has long been fundamental in physical theory. The classical field theories of gravitation and electromagnetism were evolved, as rational alternatives to theories of action at a distance, to account for the transmission of information by gravity and electrical action between different points of space and time. The first applications of the Principle of Least Action were to the mechanics of particles and rigid bodies, but were easily extended to embrace theories of the gravitational and electromagnetic field. In the twentieth century, new field theories were developed on the basis of Schrödinger's wave mechanics and other wave equations for particles of every type, so that field theory became the natural medium for the formulation of the fundamental laws of physics.

The need for the quantization of the electromagnetic field was recognized in the first formulation of quantum mechanics by Born and Jordan, and systematic methods for the quantization of fields were soon developed by Heisenberg and Pauli. The first formulations of quantum electrodynamics used non-relativistic techniques, and a perturbation theory based on expansions in powers of the fine-structure constant $\alpha = e^2/(4\pi\hbar c)$, with e in Heaviside units. Though successful in the first approximation of perturbation theory, they led to divergent and therefore meaningless results in higher approximations. The possibility of obtaining finite and meaningful results to all orders of perturbation theory was opened with the development of systematic renormalization methods, manifestly consistent with the special theory of relativity, by Tomonaga, Schwinger, Feynman and Dyson, and led to the development of non-perturbative methods by Kallén, Schwinger and others. The extension of the methods of quantum electrodynamics to theories of the weak and strong interactions with gauge groups of Yang-Mills type followed naturally, but highlighted the problem of the natural diversity of the elementary particles, which appears to be closely related to the choice of gauge group. The extension of the special relativistic methods to include gravitation has also proved a difficult task. There are several promising approaches, of which string theory is the nearest to the mainstream of quantized field theory and will be considered briefly in the final section of this chapter.

In classical physics, the field variables were functions of coordinates representing position and time, and satisfied differential equations with boundary conditions usually determined by a distribution of sources. In the early years of the development of the quantized theories, the principal innovation was that the field variables were treated as matrices, but it also became important to derive the differential equations from the Principle of Least Action in order to obtain an unambiguous formulation of the commutation relations satisfied by the matrices. The present approach to quantized field theory is similar, but is more strongly influenced by information theory. A quantized field variable $\varphi(x)$ is not in general an observable, but a function of the space-time coordinates (x^0, x^1, x^2, x^3) adopted by an observer. The fundamental observables can be constructed from the field variables, which are therefore necessarily associated with an inertial frame in which the measurement of the fundamental observables may be made. The differential equations satisfied by the field variables are normally the same as in the the unquantized theories, as might be expected from the fact that they result from the need to relate observations made in different inertial frames. But, as a consequence of quantization, a field is ultimately interpreted as providing a representation of the transmission of information though space and time by particles of the same type but possibly different momenta. The most natural applications of field theory are to elementary particles such as electrons and photons, but there are also useful applications to composite systems, irrespective of whether the details of their internal structure are to be taken into consideration.

An hermitean field variable may be considered to be an observable, but most field variables, including those representing charged particles, are not hermitean. Where a field variable $\varphi(x)$ is not hermitean, it represents *absorption (annihilation) of particles* of a particular type, and the *creation of antiparticles* of the same type, whereas its hermitean conjugate $\varphi^\dagger(x)$ is also a field variable and represents the creation of particles and the absorption of antiparticles of the same type. With some notable exceptions such as the photon, most particles have antiparticles: the positron, for instance, is the antiparticle of the electron.

The inevitable features of elementary particles are their their existence, their type, and their relation to the observer. The existence or non-existence at a particular time of particles of a particular type is determined by creation and annihilation matrices of the type discussed in Sects. 2.1 and 4.3 for fermions, or in Sect. 4.4 for bosons. A field variable $\varphi_v(x)$ associated with particles of a particular type v is therefore a matrix expressible in terms of these creation and annihilation matrices. The analogy with classical field theory is best preserved in the *Heisenberg representation*, where the statistical matrix $P(0)$ is that of a fixed observational system at the origin of coordinates. As in (5.53), we therefore set $P(x) = U(x)P(0)U^\dagger(x)$, so that the expectation value of any function $F[\varphi_v(x)]$ of the field variables becomes

$$\langle [F(\varphi(x)]] \rangle = \mathrm{tr}\{F[\varphi(x)]P(0)\}, \tag{6.1}$$

and is obviously a function of the coordinates. In the present chapter, *we shall consider inertial frames differing in time and position but with the same orientation, velocity and other parameters*, so that the total energy, momentum and angular momentum commute with $U(x)$ and have the same value in all inertial frames:

$$E(x) = U^\dagger(x)EU(x) = E,$$

$$\mathbf{K}(x) = U^\dagger(x)\mathbf{K}U(x) = \mathbf{K}, \qquad \mathbf{J}(x) = U^\dagger(x)\mathbf{J}U(x) = \mathbf{J}.$$

On the other hand, according to (5.58) and (6.1), the field variables satisfy the relations

$$\mathrm{i}\hbar\frac{\partial\varphi_v(x)}{\partial t} = [\varphi_v(x), E], \qquad -\mathrm{i}\hbar\frac{\partial\varphi_v(x)}{\partial \mathbf{x}} = [\varphi_v(x), \mathbf{K}].$$

At this point we shall, however, simplify the notation by taking units in which the velocity of light $c = 1$, so that writing $t = x^0$, $E = K^0$ and

$$\mathrm{i}\hbar\varphi_{v,\lambda}(x) = \mathrm{i}\hbar\frac{\partial\varphi_v(x)}{\partial x^\lambda} = [K_\lambda, \varphi_v(x)] \tag{6.2}$$

for $\lambda = 0, 1, 2, 3$, so that as a subscript , λ denotes partial differentiation with respect to x^λ. For field variables in the Heisenberg representation, these equations express the universal requirement that the total energy and momentum of a system should be generators of translations in space and time; they are of course not valid in the Schrödinger representation. When the energy and momentum have been expressed in terms of the field variables, (6.2) *will be used to determine the commutation relations of the fields.*

We now consider in a preliminary way the application to field theory of the Principle of Least Action. It is often convenient to expand the field variables $\varphi_v(x)$ at any time t in terms of a complete set of numerical functions $f_k(\mathbf{x})$ of position within a finite region $R = R(t)$, thus:

$$\varphi_v(x) = \sum_k q_{kv} f_k(\mathbf{x}). \tag{6.3}$$

If, for instance, the region is rectangular and of volume V, $f_k(\mathbf{k}) = \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{x}/\hbar)/(\hbar^3 V)^{\frac{1}{2}}$ and this is a Fourier expansion, but in general the complex coefficients q_{kv} are used to specify the state of the system, as in (1.4); in a quantized theory they are matrices which will be subsequently interpreted as creation and annihilation matrices. The action within a region Ω of space and time can then be expressed, as in (1.2), as the integral with respect to time of a Lagrangian function $L(q_{kv}, \dot{q}_{kv})$, or, equivalently, as the integral over Ω of a Lagragian density $\mathcal{L}(\varphi_v, \varphi_{v,\lambda})$ depending on the field variables $\varphi_v = \varphi_v(x)$ and their space-time derivatives $\varphi_{v,\lambda} = \varphi_{v,\lambda}(x)$ in the Heisenberg representation, thus:

$$A = \int L(q_{vk}, \dot{q}_{vk})dt = \int_\Omega \mathcal{L}(\varphi_v, \varphi_{v,\lambda})d^4x, \tag{6.4}$$

where both integrations are restricted to the region Ω of space-time on which the action is defined.

The differential equations satisfied by the field variables are obtained in the usual way by requiring that the action should have its minimum, when the φ_v have fixed values on the boundary of Ω. If

$$\rho^v \equiv \frac{\partial \mathcal{L}}{\partial \varphi_v}, \qquad \pi^{v\lambda} \equiv \frac{\partial \mathcal{L}}{\partial \varphi_{v,\lambda}} \tag{6.5}$$

and $\delta\varphi_v(x)$ denotes an arbitrary small variation in $\varphi_v(x)$ within Ω, this minimum is given by

$$\delta A = \int_\Omega (\rho^v \delta\varphi_v + \pi^{v\lambda}\delta\varphi_{v,\lambda}) d^4x$$

$$= \int_\Omega [(\rho^v - \pi^{v\lambda}_{\ ,\lambda})\delta\varphi_v + (\pi^{v\lambda}\delta\varphi_v)_{,\lambda}] d^4x, \tag{6.6}$$

where the summation convention is applied to v as well as to all greek affixes. The last term can be converted to an integral over the three-dimensional boundary Σ of Ω, thus:

$$\int_\Omega (\pi^{v\lambda}\delta\varphi_v)_{,\lambda} d^4x = \int_\Sigma \pi^{v\lambda}\delta\varphi_v d\Sigma_\lambda.$$

But $\delta\varphi_v = 0$ on the boundary and $\delta\varphi_v$ is arbitrary within Ω, so it follows from (6.6) that

$$\pi^{v\lambda}_{\ ,\lambda} = \rho^v, \qquad \text{i.e.,} \qquad \frac{\partial}{\partial x^\lambda}\frac{\partial \mathcal{L}}{\partial \varphi_{v,\lambda}} = \frac{\partial \mathcal{L}}{\partial \varphi_v}. \tag{6.7}$$

These are the *field equations* which must be satisfied by the field variables. The $\pi^{v\lambda}$ are called *conjugate field variables* and play a part in field theory analogous to the p_k in (1.6).

*By integrating the field equations over the region $R(t)$ within Ω at time t, it can be verified that they are equivalent to the Lagrangian equations (1.8) satisfied by the q_{vk} in (6.3) and (6.4).

A canonical *energy–momentum tensor density* $\mathcal{K}^\mu_\lambda$ can also be obtained by variation of the action, but in this instance the variation is assumed to be consistent with the field equations and due to a displacement δx^λ of the three-dimensional boundary Σ of Ω, keeping the actual values of the φ_v on the boundary fixed. Then, if $\delta\varphi_v(x)$ is the variation of the value of $\varphi_v(x)$ at any point x^λ on the undisplaced boundary,

$$\delta\varphi_v(x) + \varphi_{v,\lambda}(x)\delta x^\lambda = 0, \tag{6.8}$$

and the change in the action is

$$\delta A = \int_\Omega (\rho^v \delta\varphi_v + \pi^{v\mu}\delta\varphi_{v,\mu}) d^4x + \int_\Sigma \mathcal{L}\delta x^\lambda d\Sigma_\lambda.$$

If we substitute for ρ^v from the field equations (6.7), the first integrand becomes $(\pi^{v\mu}\delta\varphi_v)_{,\mu}$, so that the integral over Ω can be converted to an integral over the boundary, and with the help of (6.8) we obtain

$$\delta A = -\int \mathcal{K}^\mu_\lambda \delta x^\lambda d\Sigma_\mu, \qquad \mathcal{K}^\mu_\lambda = -\mathcal{L}\delta^\mu_\lambda + \sum_v \pi^{v\mu}\varphi_{v,\lambda}. \tag{6.9}$$

When this result is compared with (5.57), it becomes evident that the total energy and momentum in the three dimensional region $R = R(t)$ contained with Ω at time t is

$$K_\lambda = \int_R \mathcal{K}^0_\lambda d^3x \tag{6.10}$$

so that the component $\mathcal{K}^0_0$ of the tensor $\mathcal{K}^\mu_\lambda$ is the energy density, and $(\mathcal{K}^0_1, \mathcal{K}^0_2, \mathcal{K}^0_3)$ are the cartesian components of the momentum density.

Since $\mathcal{L}_{,\lambda} = \rho^v\varphi_{v,\lambda} + \pi^{v\lambda}\varphi_{v,\lambda,\mu}$, the tensor satisfies the *conservation equations*

$$\mathcal{K}^\mu_{\lambda,\mu} = -\mathcal{L}_{,\lambda} + \pi^{v\mu}_{\ ,\mu}\varphi_{v,\lambda} + \pi^{v\mu}\varphi_{v,\lambda,\mu} = 0, \tag{6.11}$$

from which it can be inferred, by integration over the region R, that

$$\frac{dK_\lambda}{dt} = -\int_S \mathcal{K}^\alpha_\lambda dS_\alpha,$$

where the affix α takes only the values 1, 2 and 3 and (dS_1, dS_2, dS_3) are cartesian components of a element $d\mathbf{S}$ of the two-dimensional surface S of R. This may be interpreted as meaning that any change with time of the component K_λ of the energy–momentum vector can be attributed to a flux through the surface of the region, so that the components $(\mathcal{K}^1_\lambda, \mathcal{K}^2_\lambda, \mathcal{K}^3_\lambda)$ of the energy–momentum tensor density are *flux densities*. It also follows that if the region R within Ω at time t is so large that there is no flux across its surface, the total energy and momentum of the fields does not change with time.

6.1 Free Field Theories

In the present section we shall be concerned only with the simplest applications, to the theory of fields representing freely propagating particles, and shall not therefore consider the interaction of fields of different types. It will be shown, however, in the next section that the free field theories play an essential role in the theory of fields in interaction.

There are two principal types of fields, representing fermions and bosons respectively, which need to be quantized in different ways, but their field

theories are similar when the field equations are reduced to linear form. For bosons or fermions with a given mass and spin, the field variables φ_v reduce to components ψ_v and $\bar{\psi}^v$ of a vector ψ and a conjugate vector $\bar{\psi}$, which in a quantized theory are treated as matrices. The field equations satisfied by these vectors are

$$\mathrm{i}\hbar\alpha^\lambda\psi_{,\lambda} - sm\psi = 0, \qquad \mathrm{i}\hbar\bar{\psi}_{,\lambda}\alpha^\lambda + \bar{\psi}sm = 0, \tag{6.12}$$

in units with $c = 1$, where m is the mass, and $2s$ the maximum value of the spin. These equations are quantized versions of those introduced in (4.11), and the α-matrices are related by $\alpha^\lambda = \frac{1}{2}\gamma^\lambda$ to the Dirac matrices γ^λ for fermions of spin $\frac{1}{2}$ or by $\alpha^\lambda = \beta^\lambda$ to the Kemmer matrices β^λ for bosons of spin 0 or 1. Although ψ and $\bar{\psi}$ are to be treated as independent field variables, they are related by a conjugation of the type

$$\bar{\psi} = \psi^\dagger\eta, \qquad \eta^2 = 1, \qquad (\alpha^\lambda)^\dagger = \alpha_\lambda = \eta\alpha^\lambda\eta, \tag{6.13}$$

where † as usual denotes the hermitean conjugate, and the second equation of (6.12) then follows from the first. In fact, the second and third of these equations are satisfied if $\eta = \gamma_0$ when $\alpha^\lambda = \frac{1}{2}\mathrm{i}\gamma^\lambda$ and $\eta = 2{\beta_0}^2 - 1$ when $\alpha^\lambda = \mathrm{i}\beta^\lambda$; a general for η was given in (4.12). From the field variable ψ and its adjoint $\bar{\psi}$ a four-vector *particle current density*

$$i^\lambda = \bar{\psi}\alpha^\lambda\psi \tag{6.14}$$

can be constructed, which, by virtue of the field equations (6.12), satisfies the conservation equation

$$i^\lambda{}_{,\lambda} = \bar{\psi}_{,\lambda}\alpha^\lambda\psi + \bar{\psi}\alpha^\lambda\psi_{,\lambda} = 0.$$

The field equations are consistent with (6.5) and (6.7) if we adopt the Lagrangian density

$$\mathcal{L} = \tfrac{1}{2}\,\mathrm{i}\hbar(\bar{\psi}\alpha^\lambda\psi_{,\lambda} - \bar{\psi}_{,\lambda}\alpha^\lambda\psi) - \bar{\psi}sm\psi, \tag{6.15}$$

since then

$$\pi^\lambda = \partial\mathcal{L}/\partial\psi_{,\lambda} = \tfrac{1}{2}\,\mathrm{i}\hbar\bar{\psi}\alpha^\lambda, \qquad \rho = \partial\mathcal{L}/\partial\psi = -\tfrac{1}{2}\mathrm{i}\hbar\bar{\psi}_{,\lambda}\alpha^\lambda - \bar{\psi}sm,$$

$$\bar{\pi}^\lambda = \partial\mathcal{L}/\partial\bar{\psi}_{,\lambda} = -\tfrac{1}{2}\hbar\alpha^\lambda\psi, \qquad \bar{\rho} = \partial\mathcal{L}/\partial\bar{\psi} = \tfrac{1}{2}\,\hbar\alpha^\lambda\bar{\psi}_{,\lambda} - sm\psi. \tag{6.16}$$

Solutions of the field equations (6.12) for ψ and $\bar{\psi}$ are obtained in simplest form within a region R which is a rectangular box with sides L_1, L_2 and L_3 so that the volume is $V = L_1L_2L_3$. Then the most general solutions for $\psi(x)$ and $\bar{\psi}(x)$ are obtained from a set of independent solutions $\psi_k(x)$ and $\bar{\psi}_k(x)$, thus:

$$\psi(x) = \sum_k c_k\psi_k(x), \qquad \bar{\psi}(x) = \sum_k c_k^\dagger\bar{\psi}_k(x), \tag{6.17}$$

where the subscript k represents not only the energy–momentum k^λ, but eigenvalues of the spin, and possibly other observables, allowed by the components $\psi_v(x)$ and $\bar{\psi}_v(x)$ of the field variables. The coefficients c_k and their hermitean conjugates $c_k^\dagger$ are matrices that will later be identified as *creation and annihilation matrices* for particles or antiparticles with the energy–momentum k^λ and the other observables with eigenvalues denoted by k. *The individual terms of the Fourier expansions in (6.17) are therefore identified with factors of a countably infinite set of qubits which form a 'tape' representing the information to be gained from the detection of the individual particles represented by the field.*

As each term $\psi_k(x)$ of the expansion of $\psi(x)$ in (6.17) is an appropriately normalized solution of the free field equation, it can be expressed as a product of the wave function $e_k(x)$ and the vector ζ_k defined by

$$\psi_k(x) = \zeta_k e_k(x), \qquad e_k(x) = \mid V \mid^{-\frac{1}{2}} \exp(-\mathrm{i}k_\mu x^\mu/\hbar),$$

$$\alpha^\lambda k_\lambda\zeta_k = sm\zeta_k, \qquad \bar{\zeta}_k\alpha^0\zeta_k = s. \tag{6.18}$$

The summation in (6.17) is over all numerical four-vectors k_μ such that the $k_\alpha L_\alpha/(2\pi\hbar)$ (for $\alpha = 1, 2, 3$) are integers, but also over the spin states parallel or anti-parallel to the direction of the momentum.

With α^λ defined as in (6.12), it follows from the third of the equations (6.18) that

$$k^\lambda k_\lambda = k_0^2 - \mathbf{k}^2 = m^2, \qquad k_0 = \pm(\mathbf{k}^2 + m^2)^{\frac{1}{2}}.$$

Energy and momenta satisfying this condition, which is satisfied only in free field theories, are said to on the *mass shell*. As there are two values of $k_0 = k^0$ satisfying the condition, differing in sign, both are included in the summation in (6.17); the positive value is associated with particles of energy k^0, and the negative value with anti-particles of energy $-k^0$, since there can be no negative energies. The coefficients $\mid V \mid^{-\frac{1}{2}}$ of the functions $e_k(x)$ are chosen so that the ortho-normality conditions

$$\int_R \bar{\psi}_k(x)\alpha^0\psi_l(x)d^3x = \mathrm{sgn}(k^0)\delta_{k,l}, \qquad \mathrm{sgn}(k^0) = k^0/\mid k^0 \mid = \pm 1 \tag{6.19}$$

are satisfied when $k^\lambda = l^\lambda$. For $\mathbf{k} \neq \mathbf{l}$, the right side vanishes because $\exp[-\mathrm{i}(\mathbf{k} - \mathbf{l})\cdot\mathbf{x}/\hbar]$ vanishes on integration over the rectangular box, and if $\mathbf{k} = \mathbf{l}$ but $k^0 = -l^0$ it follows from the third of the equations (6.18) that $\bar{\zeta}_k\alpha^0\zeta_l$, and hence the integrands of (6.19) are zero. With the help of (6.19), the creation and annihilation matrices can be expressed directly in terms of the fields variables:

$$c_k^\dagger = \mathrm{sgn}(k^0)\int_R \bar{\psi}(x)\alpha^0\psi_k(x)d^3x/s,$$

$$c_k = \mathrm{sgn}(k^0) \int_R \bar{\psi}_k(x)\alpha^0\psi(x)d^3x/s. \tag{6.20}$$

According to (6.9), the energy–momentum tensor density of the field is

$$\mathcal{K}^\mu_\lambda = -\mathcal{L}\delta^\mu_\lambda + \pi^\mu\psi_{,\lambda} + \bar{\psi}_{,\lambda}\bar{\pi}^\mu = -\mathcal{L}\delta^\mu_\lambda + \tfrac{1}{2}\mathrm{i}\hbar(\bar{\psi}\alpha^\mu\psi_{,\lambda} - \bar{\psi}_{,\lambda}\alpha^\mu\psi),$$

where the Lagrangian $\mathcal{L}$ (6.15) is found to vanish when use is made of the field equations (6.12). The expression for the energy–momentum four-vector K_λ, obtained as in (6.10) by integration of $\mathcal{K}^0_\mu$ over the region R, is therefore

$$K_\lambda = \tfrac{1}{2}\int_R \mathrm{i}\hbar(\bar{\psi}\alpha^0\psi_{,\lambda} - \bar{\psi}_{,\lambda}\alpha^0\psi)d^3x. \tag{6.21}$$

According to (6.2), we must have

$$\mathrm{i}\hbar\psi_{,\lambda}(x) = [K_\lambda, \psi(x)], \qquad \mathrm{i}\hbar\bar{\psi}_{,\lambda}(x) = [K_\lambda, \bar{\psi}(x)]. \tag{6.22}$$

The need to reconcile (6.22) with (6.21) determines the commutation relations for the field variables. The method of quantization of a field theory, in accordance with Bose–Einstein or Fermi-Dirac statistics, must be chosen to ensure the existence of a vacuum state, defined as the state of lowest energy. This depends on the spin, and we shall therefore discuss field theories with spin 0, $\frac{1}{2}$ and 1 separately in the following.

6.1.1 Spin $\frac{1}{2}$

The simplest application is to fermions of the same type and spin $\frac{1}{2}$, such as electrons. There the field variables $\bar{\psi}(x)$ and $\psi(x)$ in (6.15) are four-spinors, with components $\bar{\psi}^v(x)$ and $\psi_v(x)$ $(v = 1, 2, 3, 4)$, satisfying Dirac's equation as in Sect. 3.5, and the α^λ can therefore be replaced by $\frac{1}{2}\mathrm{i}\gamma^\lambda$, in terms of Dirac matrices. The field equations (6.12) are therefore

$$\mathrm{i}\hbar\gamma^\lambda\psi_{,\lambda} - m\psi = 0, \qquad \mathrm{i}\hbar\bar{\psi}_{,\lambda}\gamma^\lambda + \bar{\psi}m = 0 \tag{6.23}$$

Since $\eta = \gamma_0$ for spin $\frac{1}{2}$, the field variables ψ and $\bar{\psi}$ are now connected by the relation $\bar{\psi} = (\eta\psi)^\dagger = \psi^\dagger\gamma_0$, and with $\alpha^0 = \frac{1}{2}\gamma^0$ the expression (6.21) for the energy becomes

$$K_\lambda = \tfrac{1}{2}\int_R \mathrm{i}\hbar(\psi^\dagger\psi_{,\lambda} - \psi^\dagger_{,\lambda}\psi)d^3x. \tag{6.24}$$

If (6.17) is substituted into this formula, and use is made of (6.19), we obtain

$$K_\lambda = \sum_k \mathrm{sgn}(k^0)c^\dagger_k c_k k_\lambda, \tag{6.25}$$

where the subscript k is used to represent not only the energy–momentum $\pm k^\lambda$ but the spin state $\pm\frac{1}{2}$ of the fermion. There are two spin states, with

the spin parallel or antiparallel to the momentum. Anticipating that $c^\dagger_k$ and c_k are fermion creation and annihilation matrices, so that $c^\dagger_k c_k = 1 - c_k c^\dagger_k$, we can satisfy (6.22) with $\psi(x)$ expressed as in (6.17) by taking

$$[c_j, c^\dagger_k c_k] = c_k\delta_{jk} \qquad (k^0 > 0), \qquad [c_j, c_k c^\dagger_k] = c_k\delta_{jk} \qquad (k^0 < 0). \tag{6.26}$$

To ensure that the energy of the field has a lower bound, it is necessary to suppose that the particles satisfy the exclusion principle, which does not allow more than one fermion with the same spin and momentum. In this application, we therefore fulfill (6.26) with the *anti-commutation relations*

$$\{c_j, c_k\} \equiv c_j c_k + c_k c_j = 0, \qquad \{c^\dagger_j, c^\dagger_k\} \equiv c^\dagger_j c^\dagger_k + c^\dagger_k c^\dagger_j = 0,$$

$$\{c_j, c^\dagger_k\} \equiv c_j c^\dagger_k + c^\dagger_k c_j = \delta_{jk}. \tag{6.27}$$

It follows from the second of the above relations that $(c^\dagger_k)^2 = 0$, so that the creation of more than two particles with the same spin and momentum is excluded, as required. These relations are the same as those obtained for $\bar{f}_r$ and f_s in (4.39)

The expression (6.25) for the energy can be expressed in terms of fermionic qubits, thus:

$$K_\lambda = \sum_k{}'(n_k + n_{-k} - 1)k_\lambda, \qquad n_k = c^\dagger_k c_k, \qquad n_{-k} = c_{-k}c^\dagger_{-k}, \tag{6.28}$$

if the prime means that the summation $\sum'$ is restricted to energy-momenta with $k^0 > 0$. For $k^0 > 0$, the number of particles is $c^\dagger_k c_k$, but for $k^0 < 0$, the number of antiparticles is $c_k c^\dagger_k$, so that for antiparticles c_k is a creation matrix and $c^\dagger_k$ is an annihilation matrix. It follows, as we have already foreshadowed, that ψ represents the annihilation of particles and the creation of antiparticles, and $\bar{\psi}$ the creation of particles and the annihilation of antiparticles. The first two terms under the summation in (6.28) are then obviously the energy–momentum of particles and anti-particles with energy–momentum k^λ, but the the presence of the third 'zero-point' term $-k^\lambda$ is unwelcome and various methods have been proposed to eliminate it. Here we adopt what is the most realistic course by regarding it, as Dirac did, as part of the energy of the vacuum, and to recognize that experimentally only differences in energy and momentum from the vacuum are observable. We shall find that there are similar contributions to the energy–momentum of the vacuum from bosonic fields of spin 0 and 1, but with the opposite sign. It is therefore always possible to ensure that the total energy of the free fields of the vacuum is zero, by the introduction of a suitable extraneous fermionic or bosonic field.

To obtain the commutation relations satisfied by the components $\psi_u(x)$ or $\bar{\psi}^u(x)$ of the spinors $\psi(x)$ or $\bar{\psi}(x)$ at different points of space-time, we may multiply the first two equations of (6.27) by the products $\psi_{ju}(x)\psi_{kv}(x')$ or

$\bar{\psi}_{ju}(x)\bar{\psi}^v_k(x')$, and sum with respect to j and k. Then from (6.17) it follows that

$$\{\psi_u(x), \psi_v(x')\} = 0, \qquad \{\bar{\psi}^u(x), \bar{\psi}^v(x')\} = 0. \tag{6.29}$$

But to obtain the value of $\{\psi_u(x), \bar{\psi}^v(x')\}$, at least for $t = t'$, it is also necessary to make direct use of (6.22). We express K_λ in (6.24) in terms of the components of the field variables, thus:

$$K_\lambda = \tfrac{1}{2}\int_R \mathrm{i}\hbar \sum_v [\psi^{v\dagger}(x')\psi_{v,\lambda}(x') - \psi^{v\dagger}_{,\lambda}(x')\psi_v(x')]d^3x',$$

and it is then clear that, to ensure that (6.22) is satisfied, we must have

$$\{\psi_u(x), \psi^{v\dagger}(x')\} = \delta^v_u \delta_R(\mathbf{x}-\mathbf{x}') \qquad (t = t'), \tag{6.30}$$

where $\delta_R(\mathbf{x}-\mathbf{x}')$ is an analogue for the finite region R of Dirac's singular three-dimensional *delta-function* $\delta(\mathbf{x}-\mathbf{x}')$, to which it closely approximates when R is very large. It is strictly a *distribution*, whose required properties are that if $f(\mathbf{x})$ is any function of position, and $\mathbf{x}$ is in the region R, then

$$\int_R f(\mathbf{x}')\delta_R(\mathbf{x}-\mathbf{x}')d^3x' = f(\mathbf{x}),$$

$$\int_R f(\mathbf{x}')\delta_{R,\alpha}(\mathbf{x}-\mathbf{x}')d^3x' = f_{,\alpha}(\mathbf{x}) \qquad (\alpha = 1,2,3). \tag{6.31}$$

The second of these is of course a simple consequence of the first.

*It is also not difficult to verify that the third of the relations (6.27) implies (6.31).

6.1.2 Spin 0

The quantization of fields representing particles with spin 0 has an application, for example, to the field theory of the charged π-mesons of spin 0, where the π^+-meson is the antiparticle of the π^--meson. There is also a neutral π^0-meson which forms a triplet with the $\pi^\pm$-mesons, but this has a somewhat different mass and neutral particles are represented by a field variable that is real, or hermitean in a quantized theory. It is unlikely there are any elementary particles with spin 0, and a π-meson is usually assumed to be composed of a quark and an anti-quark, both of which have spin $\frac{1}{2}$. The maximum spin s in (6.12) and (6.15) is therefore given the value 1.

For spin 0 and $s = 1$ the field variables $\bar{\psi}$ and ψ are 5-vectors with components $\bar{\psi}^v$ and ψ_v ($v = 0,1,2,3,4$). Of the latter, ψ_4 is Lorentz-invariant, while the first four form a special relativistic 4-vector ψ_ρ ($\rho = 0,1,2,3$). For $s = 1$, the α-matrices reduce to Kemmer matrices ($\alpha_\lambda = \beta_\lambda$), which have the effect

$$(\beta_\lambda\psi)_\rho = g_{\lambda\rho}\psi_4, \qquad (\beta_\lambda\psi)_4 = \psi_\lambda, \tag{6.32}$$

on any vector ψ. The conjugate $\bar{\psi}$ is related to ψ by $\bar{\psi} = \psi^\dagger\eta$, where $\eta = 2\beta_0^2 - 1$ and $\eta\alpha_\lambda = \alpha^\lambda\eta$, so that

$$(\bar{\psi}\alpha^\lambda)^\rho = -\mathrm{i}(\bar{\psi}\beta^\lambda)^\rho = -\mathrm{i}g^{\lambda\rho}\bar{\psi}^4, \qquad (\bar{\psi}\alpha^\lambda)^4 = -\mathrm{i}(\bar{\psi}\beta^\lambda)^4 = -\mathrm{i}\psi^\lambda.$$

In terms of the components of the field variables, the Lagrangian density (6.15) is therefore

$$\mathcal{L} = \tfrac{1}{2}\,\mathrm{i}\hbar(\bar{\psi}^\lambda\psi_{4,\lambda} + \bar{\psi}^4\psi^\lambda_{,\lambda} - \bar{\psi}^4_{,\lambda}\psi^\lambda - \bar{\psi}^\lambda_{,\lambda}\psi_4) - \bar{\psi}^\lambda m\psi_\lambda - \bar{\psi}^4 m\psi_4, \tag{6.33}$$

and yields the field equation (6.12) for ψ in the form

$$\mathrm{i}\hbar\psi_{4,\lambda} - m\psi_\lambda = 0, \qquad \mathrm{i}\hbar\psi^\lambda_{,\lambda} - m\psi_4 = 0.$$

From these equations, it then follows that

$$\hbar^2\Box\psi_4 + m^2\psi_4 = 0, \qquad \Box\psi_4 \equiv g^{\lambda\rho}\psi_{4,\lambda,\rho}, \tag{6.34}$$

where the differential operator $\Box$ so defined is the d'Alembertian operator.

The variable ψ_4 is often denoted by $m^{\frac{1}{2}}\varphi$, and then the scalar φ also satisfies (6.34). The idea that free π-mesons should be represented by a field variable satisfying an equation of this type is due to Yukawa.

*The field equations (6.34) can also be obtained from the Lagrangian density

$$\mathcal{L} = \tfrac{1}{2}\,(\hbar^2 g^{\lambda\mu}\bar{\varphi}_{,\lambda}\varphi_{,\mu} - m^2\bar{\varphi}\varphi) \qquad (m^{\frac{1}{2}}\bar{\varphi} = \psi_4^\dagger, \qquad m^{\frac{1}{2}}\varphi = \psi). \tag{6.35}$$

The energy–momentum of the field in terms of the vectors ψ and $\bar{\psi}$ can be obtained directly from (6.21)

$$K_\lambda = \tfrac{1}{2}\int_R \mathrm{i}\hbar(\bar{\psi}\beta^0\psi_{,\lambda} - \bar{\psi}_{,\lambda}\beta^0\psi)d^3x. \tag{6.36}$$

Again we can substitute (6.17) into this result, and make use of (6.19) to obtain the same result

$$K_\lambda = \sum_k \mathrm{sgn}(k^0)c_k^\dagger c_k k_\lambda, \tag{6.37}$$

as for spin $\frac{1}{2}$ in (6.25), but now the subscript k is used only to represent the energy–momentum $\pm k^\lambda$. With the help of (6.32), (6.36) can also be expressed in terms of the components ψ_4 and $\psi_4^\dagger$ of ψ and $\psi^\dagger$, and hence in terms of $\bar{\varphi}$ and φ, thus:

$$K_\lambda = \tfrac{1}{2}\int_R (\hbar^2/m)(\psi^\dagger_{4,0}\psi_{4,\lambda} + \psi^\dagger{}_{4,\lambda}\psi_{4,0})d^3x,$$

$$=\tfrac{1}{2}\int_R \hbar^2(\bar{\varphi}_{,0}\varphi_{,\lambda}+\bar{\varphi}_{,\lambda}\varphi_{,0})d^3x \tag{6.38}$$

in agreement with the energy–momentum derived from the Lagrangian density (6.35).

We now observe that, with K_λ given by (6.37) and $\psi(x)$ by (6.17), the relations (6.22) are satisfied by

$$[c_j, c_k]=0, \qquad [c_j^\dagger, c_k^\dagger]=0, \qquad [c_j, c_k^\dagger]=\mathrm{sgn}(k^0)\delta_{k,l}. \tag{6.39}$$

For $k^0>0$ these are equivalent to the set of boson commutation relations shown in (4.49), if $\mathrm{c}_k^\dagger$ is a creation matrix and c_k is an annihilation matrix for particles of energy–momentum k^λ. For antiparticles with $k^0<0$ and energy–momentum $-k^\lambda$, however, sgn $(k^0)=-1$ and it is necessary to interpret c_k as a creation matrix and $\mathrm{c}_k^\dagger$ as an annihilation matrix. Thus, as for spin $\frac{1}{2}$, the field variable ψ is responsible for the annihilation of particles and the creation of antiparticles, whereas $\bar{\psi}$ is responsible for the creation of particles and the annihilation of antiparticles. The number of particles with energy–momentum k^λ is $N_k=c_k^\dagger c_k$, but the number of antiparticles with energy–momentum $-k^\lambda$ is $N_{-k}=c_{-k}c_{-k}^\dagger=\mathrm{c}_{-k}^\dagger c_{-k}+1$. The total energy–momentum of the field obtained from (6.37) is therefore

$$K^\lambda=\sum_k{}'(N_k+N_{-k}+1)k^\lambda, \qquad N_k=c_k^\dagger c_k, \qquad N_{-k}=c_{-k}c_{-k}^\dagger \tag{6.40}$$

where the prime attached to $\sum'$ again indicates that the summation is restricted to positive values of k^0. The first two terms under the summation are obviously the energy–momentum of particles and anti-particles with energy–momentum k^λ, and again there is a third 'zero-point' term k^λ associated with the vacuum, but with a sign opposite to that in (6.28).

To obtain the commutation relations satisfied by the components $\psi_u(x)$ or $\bar{\psi}^u(x)$ of the 5-vector $\psi(x)$ or $\bar{\psi}(x)$ at different points of space-time, we multiply the two equations of (6.29) by the products $\psi_{ju}(x)\psi_{kv}(x')$ or $\bar{\psi}_{ju}(x)\bar{\psi}_k^v(x')$, and sum with respect to j and k. Then from (6.17) it follows that

$$[\psi_u(x),\psi_v(x')]=0, \qquad [\bar{\psi}^u(x),\bar{\psi}^v(x')]=0.$$

But to obtain the non-vanishing equal-time commutators for $\psi_4(x)$ and $\bar{\psi}^v(x')$, it is easier to make use of (6.38), from which it is clear that, to ensure that (6.22) is satisfied, we must have

$$[\psi_4(x),\psi_{4,0}^\dagger(x')]=-[\psi_{4,0}(x),\psi_4^\dagger(x')]=(m/\hbar)\delta_R(\mathbf{x}-\mathbf{x}') \qquad (t=t'), \tag{6.41}$$

where $\delta_R(\mathbf{x}-\mathbf{x}')$ is again the distribution appearing in (6.31). In (6.29) we may substitute $\mathrm{i}\hbar\psi_{4,0}=m\psi_4$, the commutators of components of ψ and $\bar{\psi}$ other than $[\psi_0,\bar{\psi}_4]$ and $[\psi_4,\bar{\psi}_0]$ vanish, and since $\psi_4=m^{\frac{1}{2}}\varphi$ we obtain the *equal-time commutation relation*

$$[\varphi(x),\bar{\varphi}_{,0}^\dagger(x')]=\mathrm{i}\delta_R(\mathbf{x}-\mathbf{x}') \qquad (t=t') \tag{6.42}$$

satisfied by $\varphi(x)$.

6.1.3 Spin 1

For spin 1, the field variables $\bar{\psi}$ and ψ representing charged particles satisfy the field equations (6.12) with $s=1$:

$$\mathrm{i}\hbar\beta^\lambda\psi_{,\lambda}=m\psi, \qquad -\mathrm{i}\hbar\bar{\psi}_{,\lambda}\beta^\lambda=\bar{\psi}m,$$

where again $\beta^\lambda=\alpha^\lambda$ are the Kemmer matrices, but now in a 10-dimensional representation. Again a relation $\bar{\psi}=\psi^\dagger\eta$, with $\eta=2\beta_0^2-1$ connects ψ with its conjugate $\bar{\psi}$. Though ψ has just 10 independent components ψ_{jk} $(0\le j<k\le 4)$, or $\psi_{\rho\sigma}$ and $\psi_{\tau 4}$ $(0\le\rho<\sigma\le 3,\ 0\le\tau\le 3)$, and $\bar{\psi}$ the corresponding components $\bar{\psi}^{jk}$, or $\bar{\psi}^{\rho\sigma}$ and $\bar{\psi}^{\tau 4}$, it is convenient to write $\psi_{kj}=-\psi_{jk}$ and $\bar{\psi}_{jk}=-\bar{\psi}_{kj}$. Since

$$(\beta^\lambda\psi)_{\rho\sigma}=\delta_\rho^\lambda\psi_{\sigma 4}-\delta_\sigma^\lambda\psi_{\rho 4}, \qquad (\beta^\lambda\psi)_{\tau 4}=\psi_\tau^\lambda, \tag{6.43}$$

the field equations can be written

$$\mathrm{i}\hbar(\psi_{\sigma 4,\rho}-\psi_{\rho 4,\sigma})=m\psi_{\rho\sigma}, \qquad \mathrm{i}\hbar\psi^\lambda{}_{\tau,\lambda}=m\psi_{\tau 4}.$$

By using the second of these equations to eliminate $\psi_{\rho\sigma}$, we have

$$\Box\varphi_\tau-\partial_\tau\partial_\lambda\varphi^\lambda+m^2\varphi_\tau=0, \qquad \varphi_\tau=m^{\frac{1}{2}}\psi_{\tau 4}. \tag{6.44}$$

The field variable φ_τ is clearly a 4-vector analogue of the scalar field variable φ of (6.35), and the field theory of particles of spin 1 is often formulated in terms of φ_τ and its conjugate $\bar{\varphi}^\tau=-m^{\frac{1}{2}}\bar{\psi}^{\tau 4}$.

*From (4.15) the Lagrangian density can be obtained in the form

$$\mathcal{L}=\tfrac{1}{2}\mathrm{i}\hbar(\bar{\psi}^{\rho\sigma}\psi_{\sigma 4,\rho}-\bar{\psi}^{\sigma 4,\rho}\psi_{\rho\sigma})-\tfrac{1}{2}\bar{\psi}^{\rho\sigma}m\psi_{\rho\sigma}-\bar{\psi}^{\tau 4}m\psi_{\tau 4}, \tag{6.45}$$

and the above field equations can be derived from this in the usual way. The energy–momentum of the field is then

$$K_\lambda=\tfrac{1}{2}\int_R \mathrm{i}\hbar(\bar{\psi}^{0\mu}\psi_{\mu 4,\lambda}-\bar{\psi}^{\mu 4}_{,\lambda}\psi_{0\mu})d^3x$$

$$=\tfrac{1}{2}\int(\hbar^2/m)[(-\bar{\varphi}^{\mu,0}+\bar{\varphi}^{0,\mu})\varphi_{\mu,\lambda}+\bar{\varphi}^\tau_{,\lambda}(\varphi_{\mu,0}-\varphi_{0,\mu})]d^3x. \tag{6.46}$$

Since terms with $\mu=0$ disappear from this expression, the energy K_0 is always positive definite, and quantization in accordance with Bose statistics is appropriate. By the expansion of the field variables shown in (6.17), and

the use of the orthonormality conditions (6.19), the energy–momentum of the field can again be reduced to the form (6.37); however, for spin 1 the subscript k denotes not only the energy–momentum vector k^λ of the particles but the eigenvalues -1, 0 and $+1$ of the component $\mathbf{s}\cdot\mathbf{k}/\mid\mathbf{k}\mid$ of the spin in the direction of motion of the particle, so that the summation $\sum_k$ is over momentum and spin states. The commutation relations satisfied by the c_k and $c_k^\dagger$ have the same form as given for spin 0 in (6.39), but again the subscript k denotes both momentum and spin.

The most interesting application, and the one needed for quantum electrodynamics, is to the photon, which has zero mass and no charge, so that the field variable $\psi(x)$ representing the photon is hermitean and is therefore an 8-component spinor, satisfying the equation (4.26), with β^λ given by (4.23):

$$\mathrm{i}\beta^\lambda\partial_\lambda\psi(\kappa) = m(1+\beta_6)\psi(x),$$

$$\mathrm{i}(\beta^\lambda\psi)_{\rho\sigma} = \delta^\lambda_\rho\psi_{\sigma 4} - \delta^\lambda_\sigma\psi_{\rho 4}, \qquad \mathrm{i}(\beta^\lambda\psi)_{\tau 4} = \psi^\lambda_\tau.$$

This equation, and its conjugate, can be derived from the Lagrangian density

$$\begin{aligned}\mathcal{L} &= \tfrac{1}{2}\hbar(\bar\psi\alpha^\lambda\psi_{,\lambda} - \bar\psi_{,\lambda}\alpha^\lambda\psi) - \bar\psi m(1+\beta_6)\psi,\\ &= \tfrac{1}{2}\hbar(\bar\psi^{\rho\sigma}\psi_{\sigma 6,\rho} - \bar\psi^{\sigma 6,\rho}\psi_{\rho\sigma}) - \tfrac{1}{2}\bar\psi^{\rho\sigma}m\psi_{\rho\sigma},\end{aligned} \tag{6.47}$$

similar to (6.15), except for the disappearance of the imaginary unit, and that the mass is replaced by the matrix $m(1+\beta_6)$ which has the eigenvalue 0 on the 4-vector component $\psi_{\tau 4}$ of ψ. Also, as the photon is its own antiparticle, both $\psi_{\rho\sigma}$ and $\psi_{\tau 4}$ are assumed to be hermitean, so that ψ and $\bar\psi$ are no longer to be considered as independent field variables.

According to (4.33) and (4.35), in the usual notation derived from Maxwell's equations, $\psi_{\rho\sigma} = F_{\rho\sigma}$ is the electromagnetic field tensor with components $(F_{10}, F_{20}, F_{30}) = \mathbf{E}$ and $(F_{23}, F_{31}, F_{12}) = \mathbf{B}$ identified with the electric and magnetic field intensities, respectively, and $\psi_{\lambda 6}/m = A_{gl}$ is the four-vector potential. In this notation, the free field equations are

$$A_{\mu,\lambda} - A_{\lambda,\mu} = F_{\lambda\mu}, \qquad F^\lambda_{\mu,\lambda} = 0. \tag{6.48}$$

As already noted in Sect. 4.2, the Lorentz scalar $L = A^\lambda_{,\lambda}$ is not determined by these equations; it has no physical significance, and may be given any value. In the following we shall make the assumption that it has the value 0 in the vacuum, which is simple and sufficient, though not necessary, for the purpose of quantization.

The energy–momentum of the field can be obtained from (6.46), with the relation $\varphi^\lambda = m^{\frac{1}{2}}A^\lambda/\hbar$ to eliminate the mass and Planck's constant:

$$K_\lambda = \int_R(-A^{\mu,0} + A^{0,\mu})A_{\mu,\lambda}d^3x. \tag{6.49}$$

Again the energy is positive definite, so that quantization in accordance with Bose statistics is appropriate. The energy is also gauge invariant, since it is unchanged when $A_\lambda = A_{g\lambda}$ in a particular gauge is replaced by $A_\lambda = A_{g\lambda} + \chi_{,\lambda}$. The simplest self-consistent quantization procedure is in fact to introduce a gauge field χ, defined through the requirement that in the vacuum state the expectation value of A_λ should vanish. If, following (6.17) and (6.18), we introduce the Fourier expansions,

$$A_\lambda(x) = \sum_k c_k A_{\lambda k}(x), \quad A_{\lambda k}(x) = u_{\lambda k}e_k(x), \quad e_k(x) = \mid V\mid^{-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}k_\mu x^\mu/\hbar}. \tag{6.50}$$

Since $A_\lambda(x)$ is hermitean, $c_{-k} = c_k^\dagger$ and $u_{\lambda,-k} = u_{\lambda k}$. To reduce the energy in (6.49) to the form (6.37), we impose the normalization

$$\int_R(-k^0A^\mu_k + k^\mu A^0_k)A_{l\mu}d^3x = \mathrm{sgn}(k^0)\delta_{k,l}, \qquad -u^\lambda_k u_{\lambda k} = 1,$$

and, with the help of the boson commutation relations (6.39) this enables us to compute the equal-time commutation relations

$$[A_\lambda(x), A_\mu(x')] = [A^\lambda_{,0}(x), A^\mu_{,0}(x')] = 0,$$

$$[A^\lambda_{,0}(x), A_\mu(x')] = \mathrm{i}\delta^\lambda_\mu\delta_R(\mathbf{x}-\mathbf{x}')[-\partial^\lambda\partial_\mu\Delta_R(x-x')], \tag{6.51}$$

where

$$\Box\Delta_R(x-x') = \delta_R(\mathbf{x}-\mathbf{x}').$$

Without the bracketed term on the right side of (6.51), these relations would not be compatible with the Lorentz condition $A^\mu_{,\mu} = 0$, which most naturally determines the component A^0 of the vector potential in a Lorentz-invariant theory. As already mentioned, however, the introduction of this term may be avoided by the introduction of a gauge field, and restricting the validity of the Lorentz condition to the vacuum state.

6.2 Interacting Fields

When two or more particles represented by field variables interact, there is in general an exchange of both energy and information; and while the total energy and momentum are conserved, there is a loss of information concerning each of the particles as a result of scattering which normally involves the creation of particles not present in the initial state. Information on the existence of the particles and what happens as a result of their interaction is only recovered through the further interaction between the particles and a macroscopic detector or detectors. In field theory the processes by which this information is gained are encoded in the change with the time of the statistical matrix P of the system of particles, represented by a set of field variables

in the Heisenberg representation. The results provide a valuable framework in which elastic and inelastic scattering cross-sections, rates of decay of unstable particles, and even the energies of bound states have been calculated. We shall be interested particularly in scattering problems, where usually only two particles are present initially, but the technique is by no means limited to such problems.

It is supposed that at some initial time ($t = t_i \sim -\infty$) the particles are well separated, and have not interacted in the past, so that they are in a stationary state and their selected observables are uncorrelated. The eigenvalues of these selected observables for a particular particle will be denoted by a_k, where the subscript k is a vector representing the type of particle, as well as its energy–momentum, and the eigenvalues of other observables such as the spin. We denote the statistical matrix of the system of particles at the initial time t_i by P_i; this can be constructed from the corresponding statistical matrix P_v representing the vacuum by the application of products $C_i^\dagger$ and C_i of creation and annihilation matrices, respectively: $P_i = C_i^\dagger P_\mathrm{v} C_i$, where C_i is normalized to ensure that $\mathrm{tr}(P_i) = \mathrm{tr}(P_\mathrm{v}) = 1$. We further denote by $\nu_{i,k}$ the number of particles with selected observables a_k in the initial state, so that $\nu_{i,k}$ has the value 0 or 1 for fermions, but could have any non-negative value for bosons. If $c_k^\dagger$ and c_k are the corresponding creation and annihilation matrices for such particles (or the annihilation and creation matrices of anti-particles), according to the discussion following (4.41) a product $\mathrm{c}_k^\nu \bar{\mathrm{c}}_k^\nu$ will have the eigenvalue $\nu!$ in the vacuum state for bosons, but also for fermions, so that the statistical matrix for the system is

$$P_i = C_i^\dagger P_\mathrm{v} C_i, \qquad C_i^\dagger = \prod_k (c_k^{\nu_{i,k}})^\dagger / (\nu_{i,k}!)^{\frac{1}{2}}, \qquad C_i = \prod_k (c_k^{\nu_{i,k}}) / (\nu_{i,k}!)^{\frac{1}{2}}. \tag{6.52}$$

The vacuum state is unique in that there is, in principle, complete information concerning it: no particle can be annihilated, so that, for any k,

$$\mathrm{c}_k P_\mathrm{v} = P_\mathrm{v} c_k^\dagger = 0. \tag{6.53}$$

This means that the 'tape' representing vacuum state consists of a set of qubits, represented by idempotent matrices $n^{(r)\prime} = 1 - n^{(r)}$ or $n^{(r,j)\prime} = 1 - n^{(r,j)}$, complements of fermionic idempotents $n^{(r)}$ and $n^{(r,j)}$ of the type appearing in (4.37) and (4.47), and P_v can be expressed as a product of such matrices:

$$P_\mathrm{v} = \prod_r n^{(r)\prime} \prod_{r,j} n^{r,(j)\prime}. \tag{6.54}$$

Each of the factors of this expression, as in (2.17), is in turn factorizable into two spinor factors. The statistical matrix P_v of the vacuum state may therefore also be expressed as the outer product of two spinor factors Ψ_v and $\bar{\Psi}_\mathrm{v}$, each a countably infinite product of 2-component spinors:

$$P_\mathrm{v} = \Psi_\mathrm{v} \bar{\Psi}_\mathrm{v}, \qquad \mathrm{c}_k \Psi_\mathrm{v} = 0, \qquad \bar{\Psi}_\mathrm{v} c_k^\dagger = 0. \tag{6.55}$$

Since $\mathrm{tr}(P_\mathrm{v}) = 1$, the inner product $\bar{\Psi}_\mathrm{v}\Psi_\mathrm{v} = 1$, and $P_\mathrm{v} = g_\mathrm{v}$, a minimal projection of the same type as g_r in (1.28).

In field theory, not only the creation and annihilation matrices for individual particles in (6.52) and (6.54), but the action may be constructed from the field variables φ. For a set of interacting fields within a rectangular region Ω of space-time included between the times t_i and t, the action is the integral

$$A = \int_{t_i}^{t} L dt = \int_\Omega \mathcal{L} dt d^3x, \qquad \mathcal{L} = \sum_p \mathcal{L}^{(p)} - \mathcal{V}, \tag{6.56}$$

where L is the Lagrangian, $\mathcal{L}$ is the Lagrangian density, $\mathcal{L}^{(p)}$ the Lagrangian density of the p-th free field, and $\mathcal{V}$ the energy density arising from their interaction, assumed to depend only the field variables φ, but not on their space-time derivatives; as a term in the Lagrangian density, it is a Lorentz-invariant quantity. The interaction energy is the integral

$$V = \int_R \mathcal{V} d^3x. \tag{6.57}$$

As field theory is formulated in the Heisenberg representation, any observable O depends on the inertial frame (x) of the observer, and according to (5.60) is given by $O(x) = U^\dagger(x) O(t_i) U(x)$ in terms of its value $O(t_i) = O^\mathrm{S}$ in the inertial frame of an observer at the origin or in the Schrödinger representation. Since all observables are constructed from field variables, their values in different inertial frames are related in a similar way:

$$\varphi(x) = U^\dagger(x) \varphi(0) U(x),$$

But in considering the interaction of a set of particles, it is convenient to adopt the inertial frame of an observer at the origin in space and we shall therefore now suppose that the action depends on the time t but not on the position, orientation, velocity or other parameters of the observer. According to (5.57) we can then replace A by the time integral of the total energy E of the fields in (6.56), and the unitary matrix $U(x)$, equal to $\exp(-\mathrm{i}A/\hbar)$ in general, reduces to

$$U(t) = \exp[-\mathrm{i}E(t - t_i)/\hbar]. \tag{6.58}$$

This of course still satisfies the Schrödinger-like equation

$$\mathrm{i}\hbar \frac{dU}{dt} = EU, \qquad E = \sum_p E^{(p)} + V. \tag{6.59}$$

where $E^{(p)}$ is the energy of the r-th field, derived in the usual way from $\mathcal{L}^{(p)}$.

For $t > t_i$, the matrix U of course depends of V, but we denote its value for $V = 0$ at time t by U_0 and introduce a T-matrix by writing

$$U = U_0 T, \qquad U_0 = \exp[-\mathrm{i} \sum_p E^{(p)} (t - t_i)/\hbar],$$

so that

$$i\hbar\frac{dT}{dt} = U_0^\dagger V U_0 T = V_0 T, \qquad V_0 = U_0^\dagger V U_0 \tag{6.60}$$

As $T = 1$ at the initial time t_i, T satisfies the integral equation

$$T(t) = 1 - i\int_{t_i}^{t} V_0(t_1)T(t_1)dt_1/\hbar. \tag{6.61}$$

This equation can be solved by iteration, i.e., repeated substitution from the left into the right side, yielding

$$T(t) = 1 - i\int_{t_i}^{t} V_0(t_1)dt_1/\hbar - \int_{t_i}^{t} V_0(t_1)\int_{t_i}^{t_1} V_0(t_2)dt_2dt_1/\hbar^2 + ...$$

This is in fact the result of perturbation theory, but as the infinite series is at best semi-convergent when t is large, other methods are preferable and will be developed in the following.

Since $U_0 = 1$ and $V_0 = V(t_i)$ at the initial time t_i, the values of $V_0 = \sum_r V_{0r}g_r$ and its projections g_r at times t and t_i are related by

$$V_0(t) = T^\dagger(t)V(t_i)T(t), \qquad g_r(t) = T^\dagger(t)g_r(t_i)T(t). \tag{6.62}$$

6.2.1 The S-Matrix

When the time t becomes sufficiently large ($t \to t_f \sim \infty$), so that the interaction of the particles is complete, a new stationary state is reached, in which however the particles are not necessarily the same either in kind or number as in the initial state and, as a result of the interaction their momenta, spins, etc. are no longer uncorrelated. In this final state the matrix $T(t)$ approaches a value $S = T(t_f)$, known as the S-matrix. This is a true analogue of that defined in (5.24), because it determines the transition probabilities between the initial state and any final state of the system. To make the analogy precise, we shall now obtain a relativistic formula for its elements S_{if}, corresponding to the initial state of the particles with statistical matrix P_i and any of the possible states that may be observed at time t_f.

Of course nothing can be known about the system of particles in the absence of the detector or system of detectors placed by the observer to gain information about the interaction. This involves a further interaction between the microscopic system considered and the detecting system. As will be discussed in more detail in Sect. 8.1, the detecting system is necessarily macroscopic and consists of very many particles, and its interaction with the microscopic system must produce an observable change in its macroscopic state, which is normally a change from a metastable to a stable state. But, if and when the detecting system functions, selected information may be gained concerning the final state of the microscopic system. In a well designed experiment, information may be gained simultaneously concerning the existence,

nature and selected observables of the microscopic system in its *initial* state. The actual gain of information can only be from the macroscopic detecting system; it is not different in kind from that gained from the observation of any macroscopic event, and is always conditional on the intervention of a conscious observer.

Now, when the initial state is known in detail, it follows from (6.52) that its statistical matrix P_i admits a factorization similar to that of $P_v = \Psi_v\bar{\Psi}_v$:

$$P_i = \Psi_i\bar{\Psi}_i, \qquad \Psi_i = C_i^\dagger\Psi_v, \qquad \bar{\Psi}_i = \bar{\Psi}_v C_i. \tag{6.63}$$

The factor Ψ_i is called the *state vector* of the system for the initial state. It also satisfies the normalization condition $\bar{\Psi}_i\Psi_i = 1$, so that $\mathrm{tr}(P_i) = 1$, and $P_i = g_i$ is a minimal projective matrix.

When $t \to t_f$, T is replaced by the S-matrix in (6.62). There is a complete set of state vectors Ψ_f for the possible final states, similar in structure to the state vector Ψ_i of the initial state and normalized in a similar way: $\bar{\Psi}_f\Psi_f = 1$. Again recognizing this as an idealization, when complete information is obtained by observation concerning the particles of the final state, $g_f = \Psi_f\bar{\Psi}_f$, like $g_i = \Psi_i\bar{\Psi}_i$, is a minimal projection for the selected observables. But, according to (6.62), such projections are functions of time, and the probability that the final state represented by Ψ_f will be observed at time t_f is $p_{if} = \mathrm{tr}[g_f(t_f)P_i]$, or

$$p_{if} = \mathrm{tr}(S^\dagger g_f S g_i) = \mathrm{tr}(S^\dagger\Psi_f\bar{\Psi}_f S\Psi_i\bar{\Psi}_i) = \mid S_{if} \mid^2, \qquad S_{if} = \bar{\Psi}_f S\Psi_i. \tag{6.64}$$

For the various possible initial and final states, the S_{if} are *elements* of the S-matrix, and (6.64) makes it clear that they completely determine the transition probabilities p_{if} and hence the differential cross-section

$$d\sigma = \int_{d\Omega_{1f}}\int_{d\Omega_{2f}} ...p_{if}d^3k_{1f}d^3k_{2f}...$$

for finding the momenta of the particles in the final state in the elementary solid angles $d\Omega_{1f}$, $d\Omega_{2f}$, ...

Finally, we substitute the expression $\Psi_i = C_i^\dagger\Psi_v$ of (6.63) into (6.64), together with the similar expression $\bar{\Psi}_f = \bar{\Psi}_v C_f^\dagger$ for the conjugate vector of the final state, where $C_f^\dagger$ however involves creation matrices for time t_f, Then the elements of the S-matrix are expressed as *vacuum expectation values*:

$$S_{if} = \langle C_f S C_i^\dagger\rangle, \qquad \langle C_f S C_i^\dagger\rangle = \mathrm{tr}(C_f S C_i^\dagger P_v) = \bar{\Psi}_v C_f S C_i^\dagger\Psi_v. \tag{6.65}$$

Now, as shown in (6.20), the individual creation and annihilation matrices for the particles in the initial state (for $t = t_i$) and any final state (for $t = t_f$) can all be expressed as spatial integrals involving the corresponding field variables. The interaction energy $V_0(t)$ in (6.61) is also a function of the field variables $\varphi(x)$, so that $T(t)$ and $S = T(t_f)$ in (6.65) are expressible as time

integrals involving the corresponding field variables $\tilde{\varphi}(x)$ in the interaction representation. The elements S_{if} of the S-matrix may therefore be obtained by suitable integrations from the vacuum expectation values of products of field variables of the type

$$A_{ab...v}(x_1, x_2, ...x_l) = \langle \varphi_a(x_1)\varphi_b(x_2)...\varphi_v(x_l)\rangle. \tag{6.66}$$

These are called *amplitudes*; the field variables can be imagined as creating or annihilating particles or antiparticles at the points $x_1, x_2, ...x_l$. By comparison with the corresponding integrated expression $\langle C_f S C_i^\dagger\rangle$ in (6.65), it can be seen that the first field variables $[\varphi_a(x_1), ...]$ appearing in the vacuum expectation value are concerned with the annihilation of particles or antiparticles in the final state, the last field variables $[... , \varphi_v(x_l)]$ are concerned with the creation of particles or antiparticles in the initial state, while the remainder are derived from the S-matrix. From (6.63) and the perturbation series which follows it, it can be seen that the latter are also *in the reverse of their natural time order.*

6.2.2 Ordering in Time

The ordering of the field variables within vacuum expectation values such as (6.66) is the expression of what is known as the *Principle of Causality.* No other order is relevant to physics, and we therefore adopt the following *time ordering convention*, to be used not only within vacuum expectation values but elsewhere: any product of field variables, such as $\varphi_c(x_r)\varphi_d(x_s)$, will *mean* $\varphi_c(x_r)\varphi_d(x_s)$ if $t_r > t_s$, $\frac{1}{2}[\varphi_c(x_r)\varphi_d(x_s) \pm \varphi_d(x_s)\varphi_c(x_r)]$ if $t_r = t_s$ and $\pm\varphi_d(x_s)\varphi_c(x_r)$ if $t_r < t_s$. The negative sign is adopted to take account of the Fermi statistics, if both $\varphi_c(x_r)$ and $\varphi_d(x_s)$ are fermion fields; otherwise the positive sign is adopted. More generally, a product of any number of field variables will mean the same variables, rearranged in the reverse of their natural time order, prefixed by a negative sign if an odd permutation of fermion field variables is thereby effected. Where the times of two or more of the field variables are equal, a mean value of all permutations of those field variables is signified, again prefixed by a negative sign whenever there is an odd permutation of field variables.

*From (6.59) and (6.66) it follows that all amplitudes are translationally invariant:

$$A_{ab...v}(x_1, x_2, ...x_l) = A_{ab...v}(x_1 - x, x_2 - x...x_l - x),$$

for all x, and depend only on *differences* of the coordinates $x_1, x_2, ...x_l$. Amplitudes defined as in (6.66) were first introduced by Feynman in the context of a perturbative treatment of quantum electrodynamics, and in the following section we shall show briefly how they can be evaluated, by perturbative and non-perturbative techniques.

The time-ordering convention allows us to permute the time variables in the perturbation expansion for $T(t)$ following (6.61) which, with the corresponding expression for the S-matrix can then be rewritten in the more compact form

$$T(t) = \exp[-\mathrm{i}\int_{t_i}^{t} V_0(t_1)dt_1/\hbar], \qquad S = \exp[-\int_{t_i}^{t_f} V_0(t_1)dt_1/\hbar].$$

However, the more essential consequence is that a product $\varphi_c(x)\varphi_d(x')$ of two field variables is in general discontinuous when $t = t'$, so that if τ is any small time,

$$\int_{-\tau}^{\tau} \varphi_{c,0}(x)\varphi_d(x')dt = \{\varphi_c(x), \varphi_d(x')\},$$

$$(t = t',\ \varphi_c, \varphi_d \text{ both fermion fields}),$$

$$= [\varphi_c(x), \varphi_d(x')] \qquad (t = t', \text{ otherwise}).$$

It follows that in the neighborhood $t \approx t'$ the expression under the integral must be a multiple of the Dirac delta-function $\delta(t - t')$:

$$\varphi_{c,0}(x)\varphi_d(x') = \{\varphi_c(x), \varphi_d(x')\}\delta(t - t') \text{ or } = [\varphi_c(x), \varphi_d(x')]\delta(t - t'),$$

and more generally

$$\partial_0[\varphi_c(x)\varphi_d(x')] = \varphi_{c,0}(x)\varphi_d(x') + \{\varphi_c(x), \varphi_d(x')\}\delta(t - t'),$$

$$(\varphi_c, \varphi_d \text{ both fermion fields}),$$

$$= \varphi_{c,0}(x)\varphi_d(x') + [\varphi_c(x), \varphi_d(x')]\delta(t - t') \qquad (\text{otherwise}) . \tag{6.67}$$

This result provides some indication of the importance of equal-time commutators in field theory. Because amplitudes such as (6.66) are defined in terms of the field variables, they are related by equations which are direct consequences of the field equations, together with the equal-time commutation relations. It is also important for our purpose that *equal-time commutation relations such as (6.29), (6.30) and (6.51) are valid even if the free field is in interaction with other fields.* This can be shown quite simply by making use of the theory of the interaction representation; in (5.64), an observable O for any system S consisting of a set of interacting sub-systems was related to to its value $\tilde{O}$ in the absence of interactions by the unitary transformation $\tilde{O} = TOT^\dagger$. Observables are constructed from field variables, and if φ_a is the field variable in the presence of interaction, a corresponding field variable $\tilde{\varphi}_a$ in the interaction representation is defined by $\tilde{\varphi}_a = T\varphi_a T^\dagger$, and there is a similar relation between the creation and annihilation matrices $\tilde{c}_k^\dagger$, $\tilde{c}_k$ and $\mathrm{c}_k^\dagger$, c_k for particles represented by free and interacting fields:

$$\tilde{\varphi}_a(x) = T\varphi_a(x)T^\dagger, \qquad \tilde{c}_k^\dagger = T\mathrm{c}_k^\dagger T^\dagger, \qquad \tilde{c}_k = Tc_k T^\dagger. \tag{6.68}$$

where T depends on the time.

As the matrices $\tilde{c}_k^\dagger$, $\tilde{c}_k$ are independent of the time, the creation and annihilation matrices $c_k^\dagger$, c_k of the interacting fields depend on the time. Also, $\tilde{\varphi}_a(x)$ can be regarded as the field variable of a free field, and as equal-time commutation relations of the type

$$[\tilde{\varphi}_a(x), \tilde{\varphi}_b(x)] = [\tilde{\pi}^{a,0}(x), \tilde{\pi}^{b,0}(x')] = 0, \qquad (\tilde{\pi}^{a,0} = \partial\tilde{\mathcal{L}}/\partial\tilde{\varphi}_{a,0}),$$

$$[\tilde{\varphi}_a(x), \tilde{\pi}^{b,0}(x')] = \mathrm{i}\delta_a^b\delta(\mathbf{x}-\mathbf{x}') \qquad (t=t'),$$

or the corresponding anti-commutation relations with $[\ldots,\ldots]$ replaced by $\mathrm{i}\{\ldots,\ldots\}$, are easily converted by the use of (6.67) to similar relations involving $\varphi_a(x)$ and $\pi^{a,0}(x)$, they hold for both free and interacting fields.

*It can also be shown directly that, for fields in interaction, the equal-time commutation relations secure the consistency of (6.2) with (6.10).

6.3 Quantum Electrodynamics

The interaction of the Dirac and electromagnetic fields was the first to be studied, and provided a good indication of the difficulties which arise from the application of perturbation theory except in the first approximation. Here we shall present a more modern non-perturbative treatment, based on what are known as the Schwinger–Dyson equations, and the generalized Ward identities first given by the author.

The field variables are the Dirac spinor ψ and its conjugate $\bar{\psi} = \psi^*\gamma^0$ representing electrons and positrons, and the four-vector potential A_λ of the electromagnetic field, which is self-conjugate ($A_\lambda^\dagger = A_\lambda$). The Lagrangian density is

$$\mathcal{L} = \mathcal{L}^{(1)} + \mathcal{L}^{(2)} - \mathcal{V},$$

$$\mathcal{L}^{(1)} = \tfrac{1}{2}\,\mathrm{i}(\bar{\psi}\gamma^\lambda\psi_{,\lambda} - \bar{\psi}_{,\lambda}\gamma^\lambda\psi) - m\bar{\psi}\psi, \qquad \mathcal{L}^{(2)} = -\tfrac{1}{2}A^{\lambda,\mu}A_{\lambda,\mu}\ [+\tfrac{1}{2}A^{\lambda,\mu}A_{\mu,\lambda}]$$

$$\mathcal{V} = eA_\lambda\bar{\psi}\gamma^\lambda\psi, \tag{6.69}$$

where the term in brackets allows $\mathcal{L}^{(2)}$ to be expressed in the gauge invariant form $\frac{1}{4}F^{\lambda\mu}F_{\lambda\mu}$ and is compatible with our treatment of the electromagnetic field in the previous section, but has often been omitted. The omission was justified by the fact that its only consequence is the disappearance of a term involving $A^\lambda_{,\lambda}$ from the field equations which is arbitrary and zero if the Lorentz condition is adopted. The two constants, m and e, are identified as the 'bare' or unrenormalized mass and charge of the electron. In the quantized field theory, these constants will ultimately be replaced by 0 and Ze respectively, to take account of the generation of mass by the interaction of the electron with its own electromagnetic field and the polarization of the vacuum by the electronic charge. The field equations derived from (6.69) can be written

$$(\mathrm{i}\gamma^\lambda\partial_\lambda - m)\psi = e\gamma^\lambda A_\lambda\psi, \qquad \partial_\lambda\psi \equiv \psi_{,\lambda},$$

$$\bar{\psi}(-\mathrm{i}\bar{\partial}_\lambda\gamma^\lambda - m) = e\bar{\psi}\gamma^\lambda A_\lambda, \qquad \bar{\psi}\bar{\partial}_\lambda \equiv \bar{\psi}_{,\lambda},$$

$$\Box A_\lambda\ [-\partial_\lambda A^\mu_{,\mu}] = j_\lambda = e\bar{\psi}\gamma_\lambda\psi, \qquad \Box = \partial^2/(\partial x^\lambda\partial x_\lambda), \tag{6.70}$$

the term in brackets corresponding to that in the Lagrangian density. These are the quantized versions of Dirac's equations and Maxwell's equations, with the usual electromagnetic interactions, and j_λ is Dirac's expression for the charge-current density. It follows from (6.69) that, numerically, $\mathcal{L}^{(1)} = \mathcal{V}$, and the energy–momentum vector of the fields obtained with the help of (6.10) is

$$K_\lambda = \int [\tfrac{1}{2}\mathrm{i}(\bar{\psi}\gamma^0\psi_{,\lambda} - \bar{\psi}_{,\lambda}\gamma^0\psi) - m\bar{\psi}\psi - A^\nu_{,0}A_{\nu,\lambda} + \tfrac{1}{2}A^{\nu,\mu}A_{\nu,\mu}\delta^0_\lambda]d^3x.$$

Collecting the equal-time commutation relations from (6.29), (6.30) and (6.51), we have

$$\{\psi_c(x), \psi_d(x_1)\} = \{\bar{\psi}^c(x), \bar{\psi}^d(x_1)\} = 0, \qquad \{\psi_c(x), \psi^{d\dagger}(x_1)\} = \delta_c^d\delta(\mathbf{x}-\mathbf{x}_1),$$

$$[A_\lambda(y), A_\mu(y_1)] = [A^\lambda_{,0}(y), A^\mu_{,0}(y_1) = 0, \qquad [A^\lambda_{,0}(y), A_\mu(y_1)] = \mathrm{i}\delta^\lambda_\mu\delta(\mathbf{y}-\mathbf{y}_1). \tag{6.71}$$

On account of (6.55), the expectation values of $\psi_u(x)$, $\bar{\psi}^v(x)$ and $A_\lambda(y)$ are all zero, and the simplest non-vanishing amplitudes are

$$S_c^d(x) = \langle\psi_c(x)\bar{\psi}^d(0)\rangle, \qquad D_{\lambda\mu}(y) = \langle A_\lambda(y)A_\mu(0)\rangle,$$

$$S^d_{c\lambda}(x,y) = \langle\psi_c(x)A_\lambda(y)\bar{\psi}^d(0)\rangle, \tag{6.72}$$

of which the first two are known as the *electron propagator* and the *photon propagator* respectively. It is already clear that, because of the time-ordering convention, $D_{\mu\lambda}(y) = D_{\lambda\mu}(y)$. As a substitute for the Lorentz condition $A^\lambda_{,\lambda} = 0$, what is known as the *Landau gauge* will be adopted by assuming that

$$D^{\lambda\mu}_{,\lambda}(y) = 0, \tag{6.73}$$

but because of the time-ordering convention this condition is not without consequences, even if the Lorentz condition holds in the vacuum state; these will be investigated below.

The simplest amplitudes from which cross-sections for scattering are calculated are

$$S^{ef}_{cd}(x,x_1,x_2) = \langle\psi_c(x)\psi_d(x_1)\bar{\psi}^e(x_2)\bar{\psi}^f(0)\rangle,$$

$$S^d_{c\lambda\mu}(x,y,y_1) = \langle\psi_c(x)A_\lambda(y)A_\mu(y_1)\bar{\psi}^d(0)\rangle,$$

$$D_{\lambda\mu\nu\rho}(y,y_1,y_2) = \langle A_\lambda(y)A_\mu(y_1)A_\nu(y_2)A_\rho(0)\rangle,$$

and correspond to the scattering of two electrons or positrons by one another, the Compton scattering of a photon by an electron, and the very weak 'scattering of light by light', respectively. The first of these is also used to obtain

the energy levels and the decay constants of *positronium*, the bound state of an electron and a positron. Detailed calculations of cross-sections, decay constants and energy levels may be found in specialized books on quantum electrodynamics; here we shall obtain the fundamental relations between the amplitudes on which such calculations are based, and discuss in a general way the renormalization procedures needed to obtain finite results at all levels of perturbation theory.

The first relation connects the Dirac matrices $S(x)$ and $S_\lambda(x,y)$ with elements defined in (6.72). From the first of the field equations in (6.70), and using (6.67) to take account the effect of the differential operator $\mathrm{i}\gamma^0\partial_0$ which is part of D, we have

$$(\mathrm{i}\gamma^\lambda\partial_\lambda - m)S(x) = \langle(\mathrm{i}\gamma^\lambda\partial_\lambda - m)\psi(x)\bar\psi(0) + \mathrm{i}\gamma^0\{\psi(x),\bar\psi(0)\}\delta(t)\rangle$$

$$= e\gamma^\lambda S_\lambda(x,x) + \mathrm{i}\delta(\mathbf{x})\delta(x^0) = \mathrm{i}\delta(x) + e\gamma^\lambda S_\lambda(x,x), \qquad (6.74)$$

where $\delta(x) = \delta(\mathbf{x})\delta(x^0)$ is the *four-dimensional* delta-function whose essential property is that, if $f(x)$ is any function of the space-time coordinates x^λ, then

$$\int f(x')\delta(x-x')d^4x' = f(x).$$

For the amplitude $D_{\lambda\mu}(x)$, we have

$$D_{\lambda\mu,0}(x) = \langle A_{\lambda,0}(x)A_\mu(0)\rangle,$$

since $A_\lambda(x)$ and $A_\mu(0)$ commute when $t = 0$. So, from the last of the field equations in (6.70) and (6.73),

$$\Box D_{\lambda\mu}(x) = \langle\Box A_\lambda(x)A_\mu(0) + \mathrm{i}[A_{\lambda,0}(x), A_\mu(0)]\delta(t)\rangle eS^c_{c\lambda\mu}(x,x) + \mathrm{i}g'_{\lambda\mu}\delta(\mathbf{x})\delta(x^0)$$

$$= \mathrm{i}g'_{\lambda\mu}\delta(x) + e\mathrm{tr}[S_{\lambda\mu}(x,x)]. \qquad (6.75)$$

The results in (6.74) and (6.75) are just the simplest of a hierarchy of equations connecting amplitudes of increasing complexity. Others, beginning with

$$(\mathrm{i}\gamma^\lambda\partial_\lambda - m)S_\mu(x,y) = e\gamma^\lambda S_{\lambda\mu}(x,y,y_1), \qquad \Box_y S_\lambda(x,y) = e\mathrm{tr}_y[\gamma_\lambda S(x,y,y)],$$

$$(\mathrm{i}\gamma^\lambda\partial_\lambda - m)S_{\lambda\mu}(x,y,y_1) = \mathrm{i}\delta(x)D_{\lambda\mu}(y-y_1) + e\gamma^\lambda S_{\lambda\mu}(x,x,y,y_1), \qquad (6.76)$$

are derived in a similar way.

The simplest method of solution of these differential equations is by Fourier transformation, which also allows the interpretation of the solutions in terms of selected energy–momentum observables. The amplitudes in the momentum representation are defined by

$$S(p) = -\mathrm{i}\int S(x)\mathrm{e}^{\mathrm{i}p\cdot x}d^4x, \qquad D(k) = -\mathrm{i}\int D(y)\mathrm{e}^{\mathrm{i}k\cdot y}d^4y,$$

$$S_\lambda(p,k) = -\mathrm{i}\int\int S_\lambda(x,y)e^{\mathrm{i}(p\cdot x+k\cdot y)}d^4xd^4y, \qquad (6.77)$$

etc., where we have adopted a common practice in writing four-dimensional and Lorentz-invariant scalar products such as $p_\lambda x^\lambda$ in the form $p\cdot x$. By Fourier's integral theorem, the inverse transformations are

$$S(x) = \mathrm{i}(2\pi)^{-4}\int S(p)\mathrm{e}^{-\mathrm{i}p\cdot x}d^4p, \qquad D(y) = \mathrm{i}(2\pi)^{-4}\int D(k)\mathrm{e}^{-\mathrm{i}k\cdot y}d^4k,$$

$$S_\lambda(x,y) = \mathrm{i}(2\pi)^{-8}\int\int S_\lambda(p,k)\mathrm{e}^{-\mathrm{i}(p\cdot x+k\cdot y)}d^4pd^4k,$$

etc, and it follows, again with the help of Fourier's integral theorem, that

$$\int S_\lambda(x,x)\mathrm{e}^{-\mathrm{i}p\cdot x}d^4x$$

$$= \mathrm{i}(2\pi)^{-8}\int\int\int S_\lambda(p_1,k_1)\mathrm{e}^{-\mathrm{i}[(p_1+k_1)\cdot x - p\cdot x]}d^4p_1d^4k_1d^4x$$

$$(p_1+k_1\to p_1) \qquad = \mathrm{i}(2\pi)^{-4}\int S_\lambda(p-k_1,k_1)d^4k_1.$$

When the required space-time integrations are applied to (6.74), (6.75) and (6.76), the differential operators D and $\Box$ are replaced by $\gamma\cdot p - m$ and $-k^2 = -k\cdot k$ respectively. These are then transferred to the right side of the equations, so that if

$$S_\mathrm{F}(p) = (\gamma\cdot p - m)^{-1}, \qquad D_\mathrm{F}(k) = -k^{-2},$$

then (6.74), (6.75) and (6.76) are transformed to

$$S(p) = S_\mathrm{F}(p)[1+\Sigma(p)S(p)], \qquad \Sigma(p)S(p) = (2\pi)^{-4}e\gamma^\lambda\int S_\lambda(p-k_1,k_1)d^4k_1],$$

$$D_{\lambda\mu}(k) = D_\mathrm{F}(k)g_{\lambda\mu}[1+\Pi(k)D(k)],$$

$$\Pi(k)D(k) = (2\pi)^{-4}e\int\tfrac{1}{4}\mathrm{tr}[\gamma_\lambda S_\mu(p_1,k)]d^4p_1],$$

$$S_\lambda(p,k) = (2\pi)^{-4}eS_\mathrm{F}(p)\gamma^\mu\int S_{\mu\lambda}(p-k_1,k_1,k)d^4k_1,$$

$$S_{\lambda\mu}(p,k,k_1) = S_\mathrm{F}(p)[D_{\lambda\mu}(k-k_1)$$

$$+(2\pi)^{-4}e\gamma^\nu\int S_{\lambda\mu\nu}(p-k_2,k,k_1,k_2)d^4k_2]. \qquad (6.78)$$

The functions $S(p)$ and $D_{\lambda\mu}(k)$ are called electron and photon *propagators*, and the functions $S_\mathrm{F}(p)$ and $D_\mathrm{F}(k)$ to which they reduce when e is small, the corresponding Feynman propagators, since Feynman's discovery of their uses in his development of perturbative quantum electrodynamics. The functions

$\Sigma(p)$ and $\Pi_{\lambda\mu}(k)$ represent the emission and reabsorption of photons and pairs by electrons and photons respectively, and are called 'self-energy' effects in the literature.

From the results of (6.78) it is easy to obtain expansions of $S(p)$, $D_{\lambda\mu}(k)$ and other amplitudes as power series in e^2

$$S(p) = S_{\mathrm{F}}(p)[1 - \mathrm{i}(2\pi)^{-4}e^2 \int D_{\mathrm{F}}(k)\gamma^\lambda S_{\mathrm{F}}(p-k)\gamma_\lambda d^4k S_{\mathrm{F}}(p) + \ldots],$$

$$D(k) = D_{\mathrm{F}}(k)\{1 + (2\pi)^{-4}e \int_{\bar{4}}^{1} \mathrm{tr}[\gamma^\nu S_\nu(p_1, k)]d^4p_1\}.$$

The integrals are logarithmically divergent at high energies but it is possible to subtract the asymptotically divergent contributions, which have a rather simple structure, and absorb them into the mass and charge constants m and e in the process of 'mass and charge renormalization'. This somewhat mathematically dubious procedure can only be avoided by non-perturbative methods, which we shall follow as far a possible in this section. It is important to note that, quite apart from the divergence difficulties, care has to be taken in the integration of functions like $S_{\mathrm{F}}(x)$ and $D_{\lambda\mu}(k)$ near the singularities for $p^2 = m^2$ and $k^2 = 0$, respectively. These are given by

$$S_{\mathrm{F}}(x) = \langle \psi_{\mathrm{F}}(x)\bar{\psi}_{\mathrm{F}}(0)\rangle = -\mathrm{i}\int (\gamma\cdot p - m)^{-1}\mathrm{e}^{-\mathrm{i}p\cdot x}d^4p,$$

$$D_{\mathrm{F}}(x)g_{\lambda\mu} = \langle A_{\mathrm{F}\lambda}(x)A_{\mathrm{F}\mu}(0)\rangle = \mathrm{i}g_{\lambda\mu}\int k^{-2}\mathrm{e}^{-\mathrm{i}k\cdot x}d^4k,$$

where $\psi_{\mathrm{F}}(x)$ and $A_{\mathrm{F}\lambda}(x)$ are limiting values for small e of $\psi(x)$ and $A(x)$. Now, according to (6.53), when $t > 0$, $S_{\mathrm{F}}(x)$ represents the propagation of an electron, with positive values of p^0, from the origin to the point x^λ, but when $t < 0$ it represents the propagation of a positron, with negative values of p^0. Because of the presence of the exponential $\exp(-\mathrm{i}p^0x^0)$ in the integral, in fact only positive or negative values of p^0 will contribute to the integral $S_{\mathrm{F}}(x)$ for large positive or negative t, respectively, provided that p^0 is given a small *imaginary* part, i.e., is replaced by $p^0(1+\mathrm{i}\epsilon)$, where ϵ is arbitrary small, and this is the appropriate prescription for the evaluation of the integral. Of course, the same applies to the integral for $D_{\mathrm{F}}(x)$.

In what is known as the Landau gauge, the exact equations for the electron and photon propagators given in (6.78) can be written as the Dyson–Schwinger equations

$$S^{-1}(p) = S_{\mathrm{F}}^{-1}(p) - \Sigma(p), \qquad D^{-1}(k) = D_{\mathrm{F}}^{-1}(k) - \Pi(k),$$

$$\Sigma(p) = \mathrm{i}(2\pi)^{-4}e^2 \int \tfrac{1}{4}\gamma^\lambda D(p-p_1)S(p)\Gamma_\lambda(p,p_1)d^4p_1,$$

$$\Pi(k) = \mathrm{i}(2\pi)^{-4}e^2 \int \tfrac{1}{4}\mathrm{tr}[\gamma^\lambda S(p)\Gamma_\lambda(p, p-k)]d^4p, \tag{6.79}$$

where $\Gamma_\lambda(p, p_1)$, called the *vertex amplitude*, is defined by

$$S_\lambda(p,k) = \mathrm{i}eD(k)S(p)\Gamma_\lambda(p,p-k)S(p-k). \tag{6.80}$$

These results can be used for the development of non-perturbative solutions of the equations for the propagators and vertex amplitudes, assisted by the use of the generalized Ward identities. The simplest of these identities is most easily obtained by Fourier transformation of

$$\Box_y(\partial/\partial y^\lambda)S_\lambda(x,y) = -\mathrm{i}e(\partial/\partial y^\lambda)\langle\psi(x)\bar{\psi}(y)\gamma_\lambda\psi(y)\bar{\psi}(0)\rangle$$
$$-eS(x)\delta(x-y) + eS(x-y)\delta(x),$$

yielding

$$-k^2k^\lambda S_\lambda(p,k) = \mathrm{i}e[S(p) - S(p-k)],$$

or, on substitution from (6.80),

$$k^\lambda\Gamma_\lambda(p,p-k) = S^{-1}(p) - S^{-1}(p-k). \tag{6.81}$$

In the limit $k^\lambda \to 0$, this reduces to Ward's identity

$$\Gamma_\lambda(p,p) = (\partial/\partial p^\lambda)S^{-1}(p).$$

Although neither of these identities is sufficient to determine the vertex function uniquely in terms of the electron propagator, they can be made the basis of a variety of non-perturbative approximations to determine the functions $\Sigma(p)$ and $D(k)$ in (6.79).

With $m \neq 0$ in the field equations (6.70), the non-perturbative techniques still yield logarithmically divergent expressions affecting $\Sigma(p)$ and the normalization of the field variables. Although these divergences can be removed by renormalization, this mathematically questionable procedure is best avoided, and this is possible, at least as far as mass renormalization is concerned, in the limit $m = 0$. To achieve this limit, the inverse electron propagator is expressed in the form

$$S^{-1}(p) = \sigma(p^2)\gamma^\lambda p_\lambda - \rho(p^2)$$

with two functions $\sigma(p^2)$ and $\rho(p^2)$ which determine the physical mass of the electron as the solution of the equation $\sigma(m^2)m = \rho(m^2)$. These functions can be determined by various approximative procedures by the use of the Schwinger–Dyson equations in conjunction with the generalized Ward identities. We shall next consider the generalizations of quantum electrodynamics made possible by the use of gauge groups larger than $U(1)$.

6.4 Gauge Groups and String Theories

The success of renormalization procedures in quantum electrodynamics was no guarantee that similar methods would be successful for interacting fields in general, and successive terms in the perturbation series developed in the first theories to be developed for weak and strong interactions were in fact found to be intractably divergent. It became apparent that the success of quantum electrodynamics could be attributed to its *gauge invariance*, the fact that the Lagrangian density (6.69) was unchanged under a group of transformations of the type

$$\psi(x) \to \mathrm{e}^{\mathrm{i}e\chi(x)}\psi(x), \qquad \bar{\psi}(x) \to \mathrm{e}^{-\mathrm{i}e\chi(x)}\bar{\psi}(x), \qquad A_\lambda(x) \to A_\lambda(x) + \chi_{,\lambda}(x),$$

where $\chi(x)$ is an arbitrary differentiable function of the coordinates. The Lie group, $U(1)$ in this instance, was very simple, but suggested the possibility that any *Yang-Mills* gauge group, and its associated Lie algebra, could provide the basis of a renormalizable interacting field theory. The simplest application was to the weak interactions, which feature pairs of fermions, such as the β-particles (the electron and its neutrino), the μ-particles (the μ-meson and its neutrino) and the τ-particles (the τ-meson and its neutrino), interacting with a triplet of heavy vector bosons. These interactions were recognized as compatible with the gauge group $SU(2)$, but also suggested the possibility of a unified theory of electromagnetic and weak interactions, compatible with the broken symmetry arising from the deformation of the gauge group $SU(3)$. The strong interactions featured in a similar way triplets of fermions: quarks of various 'flavours', interacting with the set of bosons called gluons. Though these particles were not observable in isolation, the properties of the baryons and strongly interacting mesons could be accounted for reasonably well by supposing that they were made up combinations of quarks and gluons, with a symmetry associated with another gauge group $SU(3)$. Subsequent attempts were made to unify the weak, strong and electromagnetic interactions through the use of still larger gauge groups. It was evident that in the formulation of such theories, the Lie algebra associated with the gauge group should play a fundamental role.

The resulting generalization of quantum electrodynamics introduces a rather large number of fermion fields, represented by a set of Dirac spinors ψ_α and cospinors $\bar{\psi}^\beta$ $(\alpha, \beta = 1, 2...\sigma)$, interacting with boson fields, represented by a set of four-vectors A^a_λ $(a, b = 1, 2, ...)$. The latter can be used to construct a matrix

$$A_\lambda = g e'_a A^a_\lambda, \qquad [\mathrm{e}'_a, e'_b] = C^c_{ab} e'_c,$$

analogous to the electromagnetic vector potential, in which for convenience we have included a universal coupling constant g, which could be regarded as the analogue of the electric charge e. The constants C^w_{uv} are the structure constants of the Lie algebra, as defined in (A.65), and the e'_u are elements

of a Lie algebra in what is known as the adjoint representation, where the matrix elements of e'_u are $(e'_u)^w_v = C^w_{uv}$. The Lie algebra is of one of the types constructed from parafermions in Appendix A.6 and therefore expressible in terms of qubits by a formula of the type following (A.70). Present experimental information is insufficient to identify the type of Lie algebra uniquely, but the exceptional algebra E_8 is large enough to accommodate most of those which have been suggested.

The theory of the interacting fields is required to be invariant not only under the usual Lorentz transformations but also gauge transformations of the type

$$\psi_\alpha(x) \to \exp[\mathrm{i}e_a\chi^a(x)]\psi_\alpha(x), \qquad \bar{\psi}^\alpha(x) \to \exp[-\mathrm{i}e_a\chi^a(x)]\psi^\alpha(x),$$

$$A_\lambda(x) \to A_\lambda(x) + \chi_{,\lambda}(x), \qquad \chi(x) = e'_a\chi^a(x)$$

where the e_a are now elements of the Lie algebra in some representation other than the adjoint representation, and to avoid problems arising from the fact that the e_a do not commute, the components $\chi^a(x)$ of the gauge field may be assumed to be small. The elements e_a are then represented by matrices $(e_a)^\beta_\alpha$ whose action on $\psi_\alpha(x)$ and $\bar{\psi}^\alpha(x)$ is given by

$$[e_a\psi(x)]_\alpha = (e_a)^\beta_\alpha\psi_\beta(x), \qquad [\bar{\psi}(x)\mathrm{e}_a]^\alpha = \bar{\psi}^\beta(x)(\mathrm{e}_a)^\alpha_\beta.$$

The analogue of the electromagnetic field is defined by

$$F_{\lambda\mu} = A_{\mu,\lambda} - A_{\mu\lambda}$$

and the gauge-invariant Lagrangian density of the interacting fields is

$$\mathcal{L} = \mathcal{L}^{(1)} + \mathcal{L}^{(2)} - \mathcal{V},$$

$$\mathcal{L}^{(1)} = \tfrac{1}{2}\,\mathrm{i}(\bar{\psi}^\alpha\gamma^\lambda\psi_{\alpha,\lambda} - \bar{\psi}^\alpha_{,\lambda}\gamma^\lambda\psi_\alpha) - m\bar{\psi}^\alpha\psi_\alpha, \qquad \mathcal{L}^{(2)} = -\tfrac{1}{2}A^{\lambda,\mu}A_{\lambda,\mu},$$

$$\mathcal{V} = eA_\lambda\bar{\psi}\gamma^\lambda\psi. \tag{6.82}$$

In nature the exact symmetry implied by the invariance of the theory under a gauge group is broken in various ways, and must be deformed in some way. The most favoured method is due to Higgs, and requires the existence of a field or fields of spin 0 with a Lagrangian density that displaces the vacuum state as the state of lowest energy. The particles associated with these fields must have a very large mass and have not yet been observed.

6.4.1 String Theories

The most general form of quantized field theory, outlined in this section, has a Lagrangian density consistent with interactions with are *local*, in the sense that the interaction energy density $\mathcal{V}$ in (6.82) is a simple function of the

space-time coordinates x^λ. The fields are represented by hermitean or pseudo-hermitean qubits determined by the existence and selected observables of the particles of the fields. An interesting generalization may be based on the concept of particles as strings, or two-dimensional surfaces in space-time, which, as already described in Sect. 2.6, may be represented by real qubits. The structure of these strings is determined by the action, which may be related to their invariant surface area.

In the formulation of Polyakov, the action A associated with a string depends on a set of four-vector fields X^μ which are functions of the coordinates σ_α ($\alpha = 1, 2$), one space-like and the other time-like of a point on the surface of the string. The geometry of the surface is determined by a non-euclidean metric tensor $h_{\alpha\beta}$, and in these terms

$$A = -\tfrac{1}{2}T \int h^{\frac{1}{2}} h^{\alpha\beta} g_{\mu\nu} \partial_\alpha X^\mu \partial_\beta X^\nu d^2\sigma, \qquad h = -\det(h_{\alpha\beta}).$$

The fields may be quantized in accordance with Bose or Fermi statistics, and the former leads to a set of energy levels which can be interpreted as possible masses of the particle regarded as a string. String theories offer the possibility of a unification of the four known fundamental interactions of nature: the electromagnetic, weak, strong and gravitational interactions. However, in the next chapter we shall offer an interpretation of Einstein's theory of gravitation based on the informational content of the observation of the neutral particles from which our knowledge of the geometry of the universe is derived.

7. Gravitation

The Principle of Relativity requires that the fundamental laws of physics should be independent of the inertial frame of the observer. The inertial frame was supposed to be unaffected by external forces, and in the special theory of relativity this carried the implication that one inertial frame was unaccelerated relative to another. However, all observations on the earth's surface are made in the presence of forces of several different kinds. Fortunately, for most observers the strongest of these forces – the force of gravity, and the force due to contact with the earth's surface – are in approximate equilibrium with one another, and, at least over a limited area of the earth's surface, the acceleration due to gravity does not vary much and affects all forms of matter in the same way. Also, according to Newtonian theory, the gravitational force exerted by two systems of mass m_1 and m_2 on one another is

$$F = Gm_1m_2/r^2$$

at distance r, where $G \approx 6.67 \times 10^{-8}$ in cgs units, and is completely negligible in most terrestrial applications, except where one of the systems is the earth itself! From this point of view, gravity is the weakest of known forces. For these reasons, the special theory of relativity provides an adequate basis for physical phenomena in a limited region of space and time. But for larger regions in the neighborhood of massive planets and stars it is necessary to develop a generalization to take account of the variations in the gravitational field.

It will be seen from Newton's law of gravitation above that the gravitational force on any system is assumed to be proportional to its *inertial mass*, consistent with Galileo's observation that the acceleration of a system attributable to a local gravitational field is independent of its mass or its material composition. This feature has been confirmed with satisfactory accuracy by experiments, such as Eötvös' experiment, which provided a basis for the Principle of Equivalence. Einstein perceived that, as the mass of a physical system has no immediate influence on its motion under gravity, the gravitational force must be kinematical rather than dynamical, and directly related to the geometry of space-time. We shall now consider in more detail the manner in which this geometry has been evolved from the sensory and

experimentally derived information gained by centuries of human observation.

The most primitive source of geometrical information concerning the external world for any animal is through the interaction of light with the highly sensitive visual apparatus of the retina, which is connected to the cortex by a fairly complex system of optic nerves. The light consists of photons and the interaction is therefore of a quantum mechanical character, but the information conveyed by a single photon is very small and geometrical perception is the result of the accumulation of information derived from a multitude of independent visual stimuli. In early times this information was condensed into the axioms of euclidean geometry, which had nothing to do with time, but experiments with light signals eventually brought the insight that, at least locally, the geometry of the physical universe is four-dimensional and pseudo-euclidean. In the twentieth century astronomical observations of the photons transmitted from more distant sources provided the first indication that the pseudo-euclidean geometry of the special theory of relativity was also an approximation and that the de Sitter model was a better representation of the geometry of the universe. The various experimental tests of the general theory of relativity finally pointed to the influence of the distribution of matter and gravitation on the geometry of even quite small regions of space-time. But from the point of view of information theory, this geometry is constructed to a very large extent from the observation of the photons of electromagnetic radiation. Photons are electrically neutral particles, and though they are subject to scattering, quantum electrodynamics shows that they may be considered to be emitted from a definite source and subsequently absorbed without the frequent interactions suffered by charged particles. Other neutral particles, and especially the neutrinos emitted from various extraterrestrial sources, are also potential sources of information whose importance is likely to be enhanced in the future. In the present chapter we shall therefore develop a geometry of space time, consistent with a variety of cosmological models and with Einstein's theory of gravitation, but taking account of the fact that all geometrical information is derived from the observation of neutral particles.

The information gained by the detection of a single photon is conveyed by its momentum and polarization. The direction of the momentum is identified with the direction of the source, and its magnitude may provide some indication of the distance of the source, whereas the polarization is correlated with the velocity and angular velocity of the source. By the detection of a succession of photons from the same source, further information is gained concerning the velocity and acceleration of the source, and in this way the inertial system of the source and the way in which it is influenced by gravity are determined. Similar considerations apply to the detection of neutrinos, but because of the weakness of their interactions with other particles, they are much more difficult to observe than photons. Early investigations appeared to show that neutrinos had only a left-handed spin state, which is compatible

with a vanishing mass, but present experimental evidence strongly suggests that these particles, unlike photons, have a small rest-mass, consistent with an early theory of Majorana, and that they are normally but not invariably emitted and absorbed in left-handed spin states. It is not clear that a physical geometry constructed from the observation of neutrinos would be the same as that derived from the observation of light, but an informationally based theory could well provide some indication of differences which in the future could be detected experimentally.

The interpretation to be given of Einstein's law of gravitation in this chapter will therefore be in the context of a formulation of the quantum mechanics of neutral particles, generalized to take account of the curvature of space-time associated with cosmology and the gravitational field. A point of space-time will be identified with *an event* in which a neutral particle is emitted or absorbed, and the path of the particle with a *geodesic*, which, in the context of the formulation of projective geometry given in Sect. 3.1, is the *join* of the points of emission and absorption. The emission and absorption of a particle may be treated as separate events, and if the particle propagates over a distance which is large by microscopic standards the energy, momentum and helicity of the particle are selected observables. Assuming that the particle is observed, the absorber is a component of an extended detector, and with a suitable detector it is in principle possible to measure the energy–momentum polarization as well as to identify the type of the particle. Again assuming that is eventually detected and observed, the information gained includes that concerning its creation but also the selected information which is encoded in a statistical matrix. As we have seen in Sect. 6.1, in quantized field theory this information for a particular particle is represented as a component of a field variable consisting of the product of a creation or annihilation matrix $c_k^\dagger$ or c_k with a vector function of position which in the present context, restricted to neutral particles, is real and will be denoted by ζ_k. The outer product $\zeta_k\bar{\zeta}_k$ of the vector with its transpose $\bar{\zeta}_k$ will be referred to as a *relativistic density matrix* and, in keeping with the notation of Sect. 3.1, will be denoted by z_k. It is invariant under coordinate transformations and is normalized so that its trace $\mathrm{tr}(z_k) = \bar{\zeta}_k\zeta_k$ is 1. The relativistic density matrix can in principle be inferred from the states of the microscopic systems emitting and absorbing the neutral particle, which will be represented by density matrices ρ_s and ρ, respectively, following a notation introduced by Dirac.

Immediately following emission, the relativistic density matrix z_s at the source of the particle is strongly correlated with, even if not determined by, the density matrix ρ_s of its microscopic emitter; the latter is normally a component of a more extended system of particles. In a similar way, in the process of absorption, the relativistic matrix z of the particle becomes strongly correlated with the density matrix ρ of its microscopic absorber. In this way the relativistic density matrix provides information concerning not only the particle itself but the direction and other characteristics of its

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source. In the following, we shall show how the geometry of space-time may be constructed from this and similar information. The points of this geometry are the events associated with the emission and absorption of neutral particles, and when such a point is represented by a relativistic density matrix z, a non-euclidean geometry may be constructed to contain this point and the points representing a multitude of other events.

7.1 Geometry in Terms of Quantal Information

In the preceding discussion, the selected vector ζ from which the relativistic density matrix $z = \zeta\bar{\zeta}$ is constructed has been identified as representing the information concerning a neutral particle. But since field theory provides the generally accepted basis for the representation of information concerning particles of all kinds, we shall begin with a brief formulation of the field theory of free particles, and in particular of the photons and neutrinos which we have identified as the primary sources of geometrical information. In the context of the special theory of relativity, the field theory of free particles has been developed in some detail in Sect. 6.1, but here we shall be concerned specifically with a field variable ψ representing neutral particles and shall attempt to formulate a field equation for ψ which is independent of the spin. The validity of this field equation will again be restricted to the special theory of relativity, but later in this chapter it will be generalized to take account of cosmological and gravitational effects.

To begin with, we consider the neutrino, which has spin $\frac{1}{2}$. Assumed to have non-vanishing rest mass, it cannot be identical with its anti-particle, and has two states with different helicity, an observable with the value -1 in the dominant left-handed states and $+1$ in the rare right-handed states. The field variable ψ is responsible not only for the annihilation of neutrinos but the creation of anti-neutrinos, which have the same mass but the opposite helicity. To provide for states of different helicity, we replace the mass m in Dirac's equation (6.23) for the electron by a matrix $m\tau$, where τ is an helicity conjugation matrix, so that the field equation in the interaction representation becomes

$$\mathrm{i}\gamma^\lambda\psi_{,\lambda} = m\tau\psi, \qquad \psi_{,\lambda} = \frac{\partial\psi}{\partial x^\lambda}, \qquad (\lambda = 0,1,2,3). \tag{7.1}$$

Here and in the following units are chosen so that $c = \hbar = 1$, where c is the velocity of light, and $2\pi\hbar$ is Planck's constant; this leaves only the unit of length unspecified. In the Majorana representation, the γ-matrices (including $\gamma_5 = \mathrm{i}\gamma^0\gamma^1\gamma^2\gamma^3$) are all imaginary, so that there are solutions ψ which are purely real or imaginary, provided that the matrix τ is real. Instead of the real and imaginary parts of solutions of Dirac's equation, ψ may be resolved into even and odd components ψ_e and ψ_o which are unchanged and change

sign, respectively, under the transformation $x^\lambda \to -x^\lambda$. We may then write $\tau = \tau_2\gamma_5$, where τ_2 is the imaginary Pauli matrix, here defined, together with τ_1 and τ_3, by

$$\tau_1(\psi_\mathrm{e},\psi_\mathrm{o}) = (\psi_\mathrm{o},\psi_\mathrm{e}), \quad \tau_2(\psi_\mathrm{e},\psi_\mathrm{o}) = \mathrm{i}(-\psi_\mathrm{o},\psi_\mathrm{e}), \quad \tau_3(\psi_\mathrm{e},\psi_\mathrm{o}) = (-\psi_\mathrm{e},\psi_\mathrm{o}). \tag{7.2}$$

It is possible for neutrinos of non-vanishing mass to exist in eigenstates of the helicity, if this is represented by the matrix $\tau_3\gamma_5$, which has eigenvalues ±1 and anticommutes with both $\gamma^\lambda$and τ.

We have already seen in Sect. 2.3 that Pauli matrices such as those appearing in (7.2) define a spinor representation of $SU(2)$ locally isomorphic with $SO(3)$. In the context of a theory of gravitation, the use of imaginaries is not appropriate, and as in Appendix A.1 we shall therefore regard the imaginary unit i as a real antisymmetric matrix similar to though distinct from τ_2. Then γ^0 is the direct product of two antisymmetric matrices, and is therefore symmetric, while the other γ^λ are antisymmetric. In the Majorana representation the matrices $\mathrm{i}\gamma^\lambda$ are in an irreducible representation of $SO(4,2)$, but, because of the introduction of the factor τ, the generalized Majorana equation (7.1) is in a representation of $SO(3)\otimes SO(4,2)$. This equation has symmetries associated with permutations of τ_1, τ_2 and τ_3, but distinct from the charge conjugation symmetries stemming from the use of the imaginary unit i in Dirac's equation. Such symmetries are naturally broken by interactions as well as by the special role of these matrices. The interchange of τ_1 and τ_3 affects the helicity of the neutrino, and even permutations could find a use in the representation of the different 'flavours' of the β-, μ- and τ-neutrinos. With this interpretation of the τ-matrices, we shall find later that in transmission over sufficiently large distances and also in a gravitational field, the mixing of different states of helicity as well as flavour is possible.

Next we consider the field equation for a photon in the interaction representation which may be written in a form similar to (7.1), but with Kemmer matrices replacing the Dirac–Majorana matrices:

$$\mathrm{i}\beta^\lambda\psi_\lambda = m\tau\psi, \qquad \psi_\mathrm{e} = (A^\lambda, F^{\mu\nu}), \qquad \psi_\mathrm{o} = (A^\lambda_\mathrm{d}, F^{\mu\nu}_\mathrm{d}). \tag{7.3}$$

where $\tau = \tau_2\beta_5$, and τ_2 is defined as in (7.2); A^λ and $F^{\mu\nu}$ are field potentials and intensities in the usual notation, and A^λ_d and $F^{\mu\nu}_\mathrm{d}$ are their duals, resulting from the interchange of electric and magnetic field variables ($\mathbf{E}_\mathrm{d} = \mathbf{B}$, $\mathbf{B}_\mathrm{d} = -\mathbf{E}$). The action of the Kemmer matrices on the 10-component vector ψ_e is given by

$$\beta^\lambda\psi_\mathrm{e} = (F^{\lambda\mu}, h^{\lambda\nu}A^\rho - h^{\lambda\rho}A^\mu), \qquad \beta_5\psi_\mathrm{e} = (0, F^{\mu\nu}_\mathrm{d}),$$

where, to distinguish it from its general relativistic counterpart, $h_{\lambda\mu}$ is now used to denote the pseudo-euclidean metric tensor with diagonal elements $(1,-1,-1,-1)$. If these substitutions are made in (7.3), the latter equation reduces to Maxwell's equations in the absence of charge, and the eigenvalue

zero of β_5 on the four-vector A^λ ensures that the mass m appears only in the relation between the intensities and the potentials, so that the mass of the photon vanishes. As usual in the interaction representation, photons with a definite spin are created by electromagnetic interactions in eigenstates of the helicity.

The interactions associated with gauge theories may result in permutation of the τ-matrices, and then other solutions of (7.3) with non-zero rest-mass can be found which could represent the neutral heavy vector boson in electroweak theories with isospin, but, because of this particle's instability, such solutions are not of interest in the present context.

7.1.1 The Relativistic Density Matrix

It deserves to be emphasised that the quantum theory of gravitation to be presented is concerned primarily with properties of neutral particles which are either observed or in principle observable; however, the effect of quite general gauge fields on these particles, including those associated with gravitation, will be taken into account in a way that is consistent with the quantization of those fields. The emission and absorption of a particle are usually in different inertial frames. According to the usual principles of quantum mechanics, the relativistic matrices z and z_s are therefore connected by a transformation which is pseudo-unitary or pseudo-orthogonal, depending on the representation:

$$z = uz_s\bar{u}, \qquad u = u_c u_g \bar{u}_c, \tag{7.4}$$

where the factors u_c and u_g represent a cosmological and gravitational transformation, respectively. The cosmological factor includes a local Lorentz transformation, responsible for aberration and the Doppler shift in the energy of the observed particle, in addition to the cosmological red shift, whereas the gravitational factor is responsible for a change of gravitational potential and the gravitational shift in frequency.

We shall begin by giving a more precise definition of the relativistic matrix z and establish a representation space for it in accordance with the procedures of quantized field theory. Within a sufficiently small region of space-time, the relativistic wave equations (7.1) and (7.3) are assumed to be valid in the interaction representation. These wave equations for a neutral particles can be generalized for any spin s in the form

$$\mathrm{i}\alpha^\lambda\psi_\lambda = m\tau\psi \tag{7.5}$$

where the α^λ-matrices are imaginary ($\frac{1}{2}\gamma^\lambda$ for spin $\frac{1}{2}$, β^λ for spin 1) and τ is the real pseudoscalar given by

$$\tau = \mathrm{i}\alpha_4, \qquad \alpha_{c+3} = \tau_c\epsilon_{\lambda\mu\nu\rho}\alpha^\lambda\alpha^\mu\alpha^\nu\alpha^\rho/(24s^3) \qquad (\mathrm{c} = 1,2,3), \tag{7.6}$$

which also defines three antisymmetric matrices anticommuting with one another, and, in the spinor representation, with the Majorana matrices as well.

There is always a real symmetric matrix η (γ_0 for spin $\frac{1}{2}$, $2\beta_0^2 - 1$ for spin 1), satisfying $\eta^2 = 1$ and commuting with α^0 but anticommuting with the other α^λ and τ, so that

$$\mathrm{i}\bar{\psi}_\lambda\alpha^\lambda = m\bar{\psi}\tau, \qquad \bar{\psi} = \psi^{\mathrm{t}}\eta, \tag{7.7}$$

where ψ^{t} is the column to row transpose of ψ. As the α^λ anticommute with τ, $\bar{\psi}\alpha^\lambda\psi$ is as usual a conserved current density.

Since the α-matrices in (7.5) are imaginary and τ in (7.2) is real, the solutions of these equations may be purely real or imaginary. They are satisfied by the field variables of quantized field theory in the interaction representation, where ψ and $\bar{\psi}$ are normally expanded in terms of a complete set of ortho-normal solutions ζ_p and $\bar{\zeta}_p$, which reduce to Fourier series within a rectangular region of volume V. Thus

$$\psi = \sum_p c_p\zeta_p/\mid p^0V\mid^{\frac{1}{2}}, \qquad \bar{\psi} = \sum_p \bar{c}_p\bar{\zeta}_p/\mid p^0V\mid^{\frac{1}{2}}, \tag{7.8}$$

where $\pm p^0$ is the (positive) energy of a created particle and c_p and $\bar{c}_p$ are creation or annihilation operators, depending on the sign of p^0. The relativistic density matrix of a neutral particle, normalized to 1, is then defined as an outer product of the type $z_p = \zeta_p\bar{\zeta}_p$, and is always real. In a cosmological context a similar expansion is possible but the rectangular region must be deformed and extended to the horizon, and the volume is then the (finite) volume of the observable universe.

But in cosmology and general relativity the equations of Dirac and Kemmer also require generalization, for charged as well as neutral particles. This is usually done by the substitution of coordinate-dependent matrices for the Dirac and Kemmer matrices. At first we shall follow this approach, and though we shall obtain a generalization of (7.5) in the final section of this chapter, for the present we simply accept the matrices α^λ and τ_c as providing the algebraic substructure of a generalized theory.

7.1.2 Representations for Arbitrary Spin

When expressed in terms of the α-matrices, the commutation relations satisfied by the elements of both the Dirac–Majorana and Kemmer algebras are

$$[\alpha_{jk}, \alpha_l] = h_{kl}\alpha_j - h_{jl}\alpha_k, \qquad [\alpha_j, \alpha_k] = \alpha_{jk}, \tag{7.9}$$

where h_{kl} is an extension of the metric tensor $h_{\lambda\mu}$ of the special theory of relativity. These relations are also applicable for any spin. Where the subscripts are restricted to values $(0,1,2,3)$, they are replaced by greek characters, so that the $\alpha_{\lambda\mu}$ are generators of a representation of the Lorentz group. But here the interpretation of the subscripts of α_{jk} and h_{jk} may be extended to include the values 4, 5 and 6 with α_4, α_5 and α_6 defined as in (7.6) and $h_{44} = h_{55} = h_{66} = -1$ in (7.9). With this extended range of subscripts, the

α_{jk} are generators of representations of $SO(6,1)$ and the α_j and α_{kl} together are generators of irreducible representations of $SO(6,2)$, within the reducible group $SO(3) \otimes SO(4,2)$ resulting from the inclusion of the τ_c. The matrices $\alpha_{\lambda 4}$ can be interpreted as generators of translations in a de Sitter space of radius R and, together with the $\alpha_{\lambda\mu}$, can be used to construct the factor u_c in (7.4). In a local region, the de Sitter space approximates very closely to the Minkowski space of special relativity. The scalar matrices α_{45}, α_{56} and α_{64} are generators of gauge transformations. The other elements $\alpha_{\lambda 5}$ and $\alpha_{\lambda 6}$ of the Lie algebra may be interpreted as generators of boosts for neutral particles and therefore have a natural role in a theory of gravitation where they will be used to construct the gauge transformation u_g in (7.4). Although these matrices do not commute exactly in general, they have projections onto the chiral states of special relativity which do so.

We have already noticed that the matrices α_λ are imaginary and τ is real in the Majorana representation, and it is quite possible for the solution ψ of (7.5) to be real. In quantized field theory it is usual to employ complex solutions which are eigenvectors of observables, such as the energy and momentum, that are represented by imaginary differential operators in the coordinate representation. But geometry, and the theory of neutral particles, are traditionally formulated in terms of real quantities, and this has been achieved in the present context by interpreting the imaginary unit as a real asymmetric matrix and the ζ_p in (7.8) are therefore real even though they are eigenvectors of the energy and momentum.

The representation of the τ_c is independent of the spin, but there are both spinor and tensor representations of the factor $SO(4,2)$ of $SO(3) \otimes SO(4,2)$. The spinor representations of $SO(4,2)$ are real analogues of the complex 4-dimensional spinor representations that are often referred to as unitary and are isomorphic with the group $SU(2,2)$, while the irreducible vector representation is 10-dimensional. As shown in the previous section, the real spinor representation may be used for neutrinos and the vector representation for photons. In the following, though we are most interested in the applications to neutrinos and photons, it will be found possible to formulate a geometrical basis for a theory of gravitation in a form which is independent of the spin and even of the representation. All of the irreducible finite-dimensional representations of $SO(4,2)$ can be obtained from spinor (Dirac or Majorana) representations by a construction similar to that used in Sect. A.6 in formulating the theory of parafermionic fields. For spin s, we may write

$$\alpha_j = \sum_{r=1}^{2s} \alpha_j^{(r)}, \qquad \alpha_{kl} = \sum_{r=1}^{2s} \alpha_{kl}^{(r)}, \tag{7.10}$$

where the $\alpha_j^{(r)}$ are in spinor representations but commute for different values of r.

The general formula for the matrix η in (7.7) is $\prod_r (2\alpha_0^{(r)})$. Any irreducible representation is characterized by its highest weight vector, whose components are the highest eigenvalues l_1, l_2 and l_3 of the commuting real symmetric matrices α_{03}, $\mathrm{i}\alpha_{12}$ and $\mathrm{i}\alpha_5$ representing the state, the spin and helicity of a neutral particle, respectively, in a particular Lorentz frame at the optical horizon. The quadratic invariant of $SO(4,2)$ is

$$\sum_{j=0}^{5} (\alpha^j \alpha_j + \sum_{\kappa=0}^{5} \alpha^{jk} \alpha_{jk}) = 2[l_2(l_2+4) + l_3(l_3+2) + l_4^2].$$

To avoid the well known problems arising from the use of more general representations, we shall later adopt representations for particles of spin s of the type used for parafermions of order $2s$, with highest weight vector $(s, s, \pm s)$, noting that the Dirac and Kemmer representations for spin $\frac{1}{2}$ and spin 1, respectively, are of this type. However, the nature of the representation will be not be needed until the final sections of this chapter, where it will appear that the state of highest weights plays a physically important part in the emission of neutral particles, in the interaction representation.

7.2 Quantum Geometry

We now describe the procedure for constructing a projective geometry of space-time in terms of the normalized density matrix of neutral particles in the coordinate representation. A point is associated with the emission or absorption of an observed particle, and is therefore represented by a relativistic density matrix z which is idempotent and minimal:

$$z^2 = z, \qquad \mathrm{tr}(z) = 1, \tag{7.11}$$

These relations are not affected by pseudo-orthogonal transformations, including gauge transformations, of the type $z \to vz\bar{v}$, under all of which z remains real and symmetric. The normalization of the trace to unity implies that z may be expressed as an outer (tensor) product of vectors ζ and $\bar{\zeta}$ of the type introduced in (7.8):

$$z = \zeta\bar{\zeta}, \qquad \bar{\zeta}\zeta = \mathrm{tr}(z) = 1, \tag{7.12}$$

where $\bar{\zeta}$ is the conjugate $\zeta^\dagger\eta$ of ζ, and $\bar{\zeta}\zeta$ denotes the corresponding inner (scalar) product. Since z is real, the factors ζ and $\bar{\zeta}$ may also be assumed to be real. When z is identified with the relativistic density matrix of an observed particle at that point, the factorization is unique except in respect of sign. It is important to note that, since the vectors are real and η is symmetric, the inner product satisfies the condition $\bar{\zeta}\zeta' = \bar{\zeta}'\zeta$.

The relations (7.12) can be written more explicitly in terms of the elements z_k^j of the matrix, and the vectorial factors ζ^j and $\bar{\zeta}_k$:

$$z_k^j = \zeta^j \bar{\zeta}_k, \qquad \zeta_k = \sum_l h_{kl}\zeta^l, \qquad \sum_j \bar{\zeta}^j \zeta_j = 1. \tag{7.13}$$

It is a matter of observational experience that with each point z of space a set of three *coordinates* (x^1, x^2, x^3) can be associated, and that in the course of time, this spatial geometry acquires a further dimension, so that a further coordinate x^0 is needed to specify the event in space and time. Any point z is then specified by the value of a matrix function $z(x)$ of the coordinates x^λ $(\lambda = 0, 1, 2, 3)$. These coordinates can be chosen in many different ways, and it was an important feature of Einstein's general theory of relativity that its validity should not be restricted to a particular system of coordinates. The factors $\bar{\zeta}$ and ζ must of course also be functions $\bar{\zeta}(x)$ and $\zeta(x)$ of the coordinates, but η_{kl} is the metric tensor of the special theory of relativity and remains independent of the coordinates. In a sufficiently small region of space-time, the variation of these functions with the coordinates can be neglected and the general theory reduces to the special theory of relativity.

As in the special theory, a join $z' \vee z$ can be associated with two points z and z', and is given by

$$z \vee z' = (z' - z)^2/s^2, \qquad \tau^2 = \tfrac{1}{2}\,\mathrm{tr}(z' - z)^2 = 1 - \mathrm{tr}(zz'). \tag{7.14}$$

where τ is the interval between z and z', imaginary if the geodesic has space-like extension. As the points z' and z are on the join,

$$z(z \vee z') = z = (z \vee z')z; \qquad z'(z \vee z') = z' = (z \vee z')z'. \tag{7.15}$$

If the points z and z' are sufficiently near to one another, the difference $z' - z$ can be treated as a differential dz, and τ^2 is replaced by

$$d\tau^2 = \tfrac{1}{2}\,\mathrm{tr}(dz^2). \tag{7.16}$$

However, z is now regarded as a function $z(x)$ of the coordinates, so that we have

$$dz = z_\lambda dx^\lambda, \qquad z_\lambda = \frac{\partial z(x)}{\partial x^\lambda}, \tag{7.17}$$

and (7.16) reduces to

$$d\tau^2 = g_{\lambda\mu} dx^\lambda dx^\mu, \qquad g_{\lambda\mu} = \tfrac{1}{2}\,\mathrm{tr}(z_\lambda z_\mu), \tag{7.18}$$

where the summation convention is to be applied to repeated Greek affixes. Comparison with (3.1) makes it clear that $g_{\lambda\mu}$ is a generalization of the metric tensor of the special theory of relativity, which for this reason is denoted by $h_{\lambda\mu}$ in the present chapter. The generalization $g_{\lambda\mu}$ now depends essentially on the x^λ, even when $h_{\lambda\mu}$ is expressed in rectangular (cartesian) coordinates. As in the special theory, the contravariant form of the metric tensor, $g^{\lambda\mu}$, is still related to $g_{\lambda\mu}$ by

$$g^{\lambda\nu} g_{\nu\mu} = \delta^\lambda_\mu, \tag{7.19}$$

with components forming the inverse of the matrix formed by $g_{\lambda\mu}$. The contravariant tensor is used to construct the contravariant form of Riemannian vectors like z_λ, thus:

$$z^\lambda = g^{\lambda\mu} z_\mu. \tag{7.20}$$

It follows from (7.13) that, if ζ_λ and $\bar{\zeta}_\lambda$, like z_λ in (7.17), are derivatives with respect to the coordinate x^λ, then $z_\lambda = \zeta_\lambda\bar{\zeta} + \zeta\bar{\zeta}_\lambda$ and $\bar{\zeta}_\lambda\zeta + \bar{\zeta}\,\zeta_\lambda = 0$. But as $\eta_{jk} = \eta_{kj}$,

$$\bar{\zeta}_\lambda\zeta = \sum_{j,k} \zeta^j_\lambda \eta_{jk} \zeta^k = \sum_{j,k} \zeta^k \eta_{kj} \zeta^j_\lambda = \bar{\zeta}\zeta_\lambda$$

and it follows that

$$\bar{\zeta}_\lambda\zeta = \bar{\zeta}\zeta_\lambda = 0, \qquad \bar{\zeta}_\lambda = \partial\bar{\zeta}/\partial x^\lambda, \qquad \zeta_\lambda = \partial\zeta/\partial x^\lambda. \tag{7.21}$$

Thus, $z_\lambda z_\mu = \zeta_\lambda\bar{\zeta}_\mu + \zeta\bar{\zeta}_\lambda\zeta_\mu\bar{\zeta}$, and with the help of (7.18), (7.19) and (7.20), we have

$$g_{\lambda\mu} = \bar{\zeta}_\lambda\zeta_\mu, \qquad z_\lambda z_\mu = \zeta_\lambda\bar{\zeta}_\mu + g_{\lambda\mu}\zeta\bar{\zeta},$$
$$\bar{\zeta}^\lambda\zeta_\mu \equiv g^{\lambda\nu}\bar{\zeta}_\nu\zeta_\mu = g^{\lambda\nu}g_{\nu\mu} = \delta^\lambda_\mu. \tag{7.22}$$

Also, if $z^{(4)} \equiv \zeta^\lambda\bar{\zeta}_\lambda = z^\lambda z_\lambda - 4z$,

$$z^{(4)2} = \zeta_\lambda\bar{\zeta}^\lambda\zeta_\mu\bar{\zeta}^\mu = \zeta_\lambda\bar{\zeta}^\lambda = z^{(4)} \tag{7.23}$$

thus $z^{(4)}$ is an idempotent, and as $\mathrm{tr}(z^{(4)}) = \delta^\lambda_\lambda = 4$, it represents a three-dimensional subspace which, however, does not contain the point z. The complementary subspace is represented by a matrix $z^{(2)}$ satisfying

$$z^\dagger = 1 - z^{(4)} = 1 - \zeta^\mu\bar{\zeta}_\mu,$$

$$z^{\dagger 2} = z^\dagger, \qquad z^\dagger z = zz^{(2)} = z, \qquad \bar{\zeta}_\lambda z^\dagger = z^\dagger\zeta_\lambda = 0. \tag{7.24}$$

These results will be needed in the following section.

7.2.1 The Curvature of Space-Time

It was an important feature of Einstein's general theory of relativity that the fundamental equations should be independent of the choice of the coordinates, and this was secured by formulating these equations in terms of *Riemannian* tensors. The simplest tensors are the invariants, that remain unchanged when the coordinates are replaced by any other coordinates x'^λ, which must of course be functions $x'^\lambda(x)$ of the x^μ. So, if w is an invariant,

$$w' = w(x') = w(x) = w. \tag{7.25}$$

In particular, the matrix z representing a point and its vectorial factors ζ and $\bar{\zeta}$ are invariants in this sense. The next simplest tensors are contravariant and covariant vectors, which transform like dx^λ and z_λ, respectively, in (7.17). If u^λ is a contravariant vector and v_λ is a covariant vector, then

$$u'^{\lambda} = \frac{\partial x'^{\lambda}}{\partial x^{\mu}} u^{\mu}, \qquad v'_{\lambda} = z_{\mu} \frac{\partial x^{\mu}}{\partial x'^{\lambda}} \tag{7.26}$$

and it is easy to verify that $u'^{\lambda} v'_{\lambda} = u^{\lambda} v_{\lambda}$, so that $u^{\lambda} v_{\lambda}$ is an invariant. The row $\bar{\zeta}_{\lambda}$ and the column ζ_{μ} in (7.21) are both covariant vectors in the sense of general relativity. To proceed further, there are contravariant, covariant and mixed tensors which transform like $u^{\lambda} u^{\mu}$, $v_{\lambda} v_{\mu}$ and $u^{\lambda} v_{\mu}$, respectively, under a change of coordinates; these are called tensors of rank 2. In general, the number of unrepeated greek affixes is the *rank* of the tensor, so that invariants and vectors are tensors of rank 0 and 1. It is clear from (7.18) and (7.19) that $g^{\lambda\mu}$, $g_{\lambda\mu}$ and δ^{λ}_{μ} must be contravariant, covariant and mixed tensors, transforming like

$$g'^{\lambda\mu} = g^{\nu\rho} \frac{\partial x'^{\lambda}}{\partial x^{\nu}} \frac{\partial x'^{\mu}}{\partial x^{\rho}}, \quad g'_{\lambda\mu} = g_{\nu\rho} \frac{\partial x^{\nu}}{\partial x'^{\lambda}} \frac{\partial x^{\rho}}{\partial x'^{\mu}}, \quad \delta'^{\lambda}_{\mu} = \delta^{\nu}_{\rho} \frac{\partial x'^{\lambda}}{\partial x^{\nu}} \frac{\partial x^{\rho}}{\partial x'^{\mu}} = \frac{\partial x'^{\lambda}}{\partial x'^{\mu}}.$$

Einstein's theory attributes gravitation to the curvature of space time, and makes use of the *Riemann–Christoffel curvature tensor* $R^{\rho}_{\lambda\mu\nu}$. We shall first state the usual definition of this tensor in terms of the *Christoffel affinity* $\Gamma^{\rho}_{\mu\nu}$:

$$\begin{aligned} R^{\rho}_{\lambda\mu\nu} &= \Gamma^{\rho}_{\lambda\nu,\mu} - \Gamma^{\rho}_{\lambda\mu,\nu} + \Gamma^{\rho}_{\sigma\mu}\Gamma^{\sigma}_{\lambda\nu} - \Gamma^{\rho}_{\sigma\nu}\Gamma^{\sigma}_{\lambda\mu}, \\ \Gamma^{\rho}_{\lambda\mu} &= \tfrac{1}{2}\, g^{\rho\nu}(g_{\nu\lambda,\mu} + g_{\nu\mu,\lambda} - g_{\lambda\mu,\nu}), \end{aligned} \tag{7.27}$$

but from (7.22) obtain simpler and equivalent definitions of the latter in terms of in terms of $\bar{\zeta}^{\rho}$ and ζ_{λ}, or in terms of the derivatives z^{ρ} and z_{λ}:

$$\Gamma^{\rho}_{\lambda\mu} = \bar{\zeta}^{\rho}\zeta_{\lambda,\mu} = -\bar{\zeta}^{\rho}_{,\mu}\zeta_{\lambda} = \tfrac{1}{2}\,\mathrm{tr}(z^{\rho} z_{\lambda,\mu}) = -\tfrac{1}{2}\mathrm{tr}(z^{\rho}_{,\mu} z_{\lambda}). \tag{7.28}$$

The above relations introduce another common notation in Riemannian analysis, which has also been adopted in earlier chapters: a subscript preceded by a comma, like $,\mu$, denotes partial differentiation with respect to the corresponding coordinate; thus $\Gamma^{\rho}_{\lambda\nu,\mu}$ means $\partial\Gamma^{\rho}_{\lambda\nu}/\partial x^{\mu}$. It should be noticed that $z_{\lambda,\mu}$ is not a covariant tensor, as it does not transform like $g_{\lambda\mu}$ in general under changes of coordinates, and it follows that $\Gamma^{\rho}_{\lambda\mu}$, in spite of its appearance, is also not a tensor. However, as we shall soon verify, $R^{\rho}_{\lambda\mu\nu}$ is a tensor of the fourth rank. Also, if we differentiate the determinant $\det(g_{\lambda\mu})$ with respect to x^{λ}, we obtain

$$\Gamma^{\mu}_{\lambda\mu} = \tfrac{1}{2}\, g^{\mu\nu} g_{\nu\mu,\lambda} = \tfrac{1}{2}\,(-g)_{,\lambda}/(-g), \qquad g = \det(g_{\lambda\mu}), \tag{7.29}$$

with the help of from (7.27) and (A.24), since $g^{\mu\nu} g$ is the cofactor of $g_{\nu\mu}$ in g.

The importance of the Christoffel affinity stems from its use in *covariant differentiation*. Thus the covariant derivative $v_{\lambda/\mu}$ of a covariant vector v_{λ} is usually defined by $v_{\lambda/\mu} = v_{\lambda,\mu} - v_{\rho}\Gamma^{\rho}_{\lambda\mu}$, but from (7.28) and (7.22) we see that

$$v_{\lambda/\mu} = v_{\mu/\lambda} = (v_{\rho}\bar{\zeta}^{\rho})_{,\mu}\zeta_{\lambda}. \tag{7.30}$$

Here $v_{\rho}\bar{\zeta}^{\rho}$ is an invariant, and $v_{\lambda/\mu}$ is therefore a covariant tensor of the second rank. In particular, if ζ_{λ} is substituted for v_{λ}, and use is made of the identity $z^{\dagger}\zeta_{\lambda} = 0$ of (7.24), where $z^{\dagger} = 1 - z^{(4)}$, we have

$$\zeta_{\lambda/\mu} = z^{(4)}_{,\mu}\zeta_{\lambda} = -z^{\dagger}_{,\mu}\zeta_{\lambda} = z^{\dagger}\zeta_{\lambda,\mu}. \tag{7.31}$$

Again using (7.24), it follows that

$$\bar{\zeta}_{\lambda/\nu}\zeta_{\mu} = \bar{\zeta}_{\lambda}\zeta_{\mu/\nu} = 0.$$

The covariant derivative is assumed to satisfy the usual chain rule for differentiation, so that

$$g_{\lambda\mu/\nu} = \bar{\zeta}_{\lambda/\nu}\zeta_{\mu} + \bar{\zeta}_{\lambda}\zeta_{\mu/\nu} = 0. \tag{7.32}$$

Using (7.28), we now evaluate

$$\Gamma^{\rho}_{\lambda\nu,\mu} - \Gamma^{\rho}_{\lambda\mu,\nu} = \bar{\zeta}^{\rho}_{,\mu}\zeta_{\lambda,\nu} - \bar{\zeta}^{\rho}_{,\nu}\zeta_{\lambda,\mu},$$

$$\Gamma^{\rho}_{\sigma\mu}\Gamma^{\sigma}_{\lambda\nu} - \Gamma^{\rho}_{\sigma\nu}\Gamma^{\sigma}_{\lambda\mu} = -\bar{\zeta}^{\rho}_{,\mu}\zeta_{\sigma}\bar{\zeta}^{\sigma}\zeta_{\lambda,\nu} + \bar{\zeta}^{\rho}_{,\nu}\zeta_{\sigma}\bar{\zeta}^{\sigma}\zeta_{\lambda,\mu},$$

so that the curvature tensor of (7.27) reduces to

$$R^{\rho}_{\lambda\mu\nu} = \bar{\zeta}^{\rho}_{,\mu} z^{\dagger}\zeta_{\lambda,\nu} - \bar{\zeta}^{\rho}_{,\nu} z^{\dagger}\zeta_{\lambda,\mu} = \bar{\zeta}^{\rho}_{/\mu}\zeta_{\lambda/\nu} - \bar{\zeta}^{\rho}_{/\nu}\zeta_{\lambda/\mu}. \tag{7.33}$$

*The formula (7.33) can also be expressed directly in terms of the matrix z:

$$R^{\rho}_{\lambda\mu\nu} = \tfrac{1}{2}\,\mathrm{tr}(\bar{z}^{\rho}_{/\mu} z_{\lambda/\nu} - \bar{z}^{\rho}_{/\nu} z_{\lambda/\mu}).$$

The covariant derivatives of ζ are defined in the usual way so as to conform with the chain rule, and the Riemann–Christoffel tensor is given by

$$\zeta_{\lambda/\mu/\nu} - \zeta_{\lambda/\nu/\mu} = \zeta_{\rho} R^{\rho}_{\lambda\mu\nu}. \tag{7.34}$$

We note that, since $g_{\lambda\mu/\nu} = 0$ and $\bar{\zeta}_{\lambda/\mu}\zeta_{\nu} = \bar{\zeta}_{\nu}\zeta_{\lambda/\mu}$, where $\zeta_{\lambda/\mu}$ is symmetric, the identity $\bar{\zeta}_{\nu}\zeta_{\lambda/\mu} = 0$ holds, and it follows that

$$R^{\rho}_{\lambda\mu\nu} = \bar{\zeta}^{\rho}(\zeta_{\lambda/\mu/\nu} - \zeta_{\lambda/\nu/\mu}) = \bar{\zeta}^{\rho}_{/\mu}\zeta_{\lambda/\nu} - \bar{\zeta}^{\rho}_{/\nu}\zeta_{\lambda/\mu}. \tag{7.35}$$

From (7.31) it is evident that this tensor can be constructed by ordinary differentiation, or by purely algebraic operations from ζ_{λ} and $z^{\dagger}_{\mu}$. Another consequence of the chain rule, together with (7.30), is that, for any vector v_{λ},

$$v_{\lambda/\mu/\nu} - v_{\lambda/\nu/\mu} = v_{\rho} R^{\rho}_{\lambda\mu\nu}. \tag{7.36}$$

Finally, we note that the tensor $R^{\rho}_{\lambda\mu\nu}$ satisfies two *Bianchi* identities:

$$\begin{aligned} R^{\rho}_{\lambda\mu\nu} + R^{\rho}_{\mu\nu\lambda} + R^{\rho}_{\nu\lambda\mu} &= 0, \\ R^{\rho}_{\lambda\mu\nu/\sigma} + R^{\rho}_{\lambda\nu\sigma/\mu} + R^{\rho}_{\lambda\sigma\mu/\nu} &= 0, \end{aligned} \tag{7.37}$$

of which the first is a direct consequence of (7.36) and the second also follows easily by covariant differentiation of (7.36) with respect to x^{σ}.

7.3 Einstein's Gravitational Field Equations

Following Einstein, we have concluded that (1) on the basis of the Principle of Equivalence, gravitation should be a kinematical and therefore geometrical, rather than dynamical, phenomenon, and (2) on the basis of the Principle of Relativity, the law of gravitation should be independent of the choice of coordinates. A formulation in terms of the Riemannian curvature tensor is therefore strongly indicated. The simplest way of meeting these requirements, and that adopted initially by Einstein, is to require the vanishing of the *Ricci tensor*

$$R_{\lambda\mu} \equiv -R^{\rho}_{\lambda\mu\rho} = \Gamma^{\rho}_{\lambda\mu,\rho} - \Gamma^{\rho}_{\lambda\rho,\mu} + \Gamma^{\rho}_{\sigma\rho}\Gamma^{\sigma}_{\lambda\mu} - \Gamma^{\rho}_{\sigma\mu}\Gamma^{\sigma}_{\lambda\rho} \tag{7.38}$$

in empty space. This law of gravitation was subsequently modified to be consistent with an approximation to de Sitter space in regions remote from large masses, so that the exact form adopted for the law of gravitation in empty space is

$$R_{\lambda\mu} = \kappa g_{\lambda\mu} \qquad (\kappa = 3/R^2), \tag{7.39}$$

where, however, the radius R of space is so large that the cosmological term on the right side of this equation may often be neglected. If we substitute from (7.32), we obtain Einstein's law, with the cosmological term, in the form

$$R_{\lambda\mu} = \bar{\zeta}^{\nu}_{/\nu}\zeta_{\lambda/\mu} - \bar{\zeta}^{\nu}_{/\mu}\zeta_{\lambda/\nu} = \kappa\bar{\zeta}_{\lambda}\zeta_{\mu}. \tag{7.40}$$

When, as in (7.38) $R_{\lambda\mu}$ is expressed in terms of the Christoffel affinity, it can be seen from (7.27) that the equations involve second derivatives of the metric tensor $g_{\lambda\mu}$, which it is supposed to determine, but although the 10 equations obtained from (7.38) with different values of λ and μ is the same as the number of components of $g_{\lambda\mu}$ there is some redundancy, because $R_{\lambda\mu}$ satisfies a set of differential equations of the first order. On setting $\sigma = \rho$ in the second of the Bianchi identities (7.37) and multiplying by $g_{\lambda\mu}$, we have

$$T^{\rho}_{\nu/\rho} = 0, \qquad T^{\rho}_{\nu} = R^{\rho}_{\nu} - \tfrac{1}{2}R^{\sigma}_{\sigma}\delta^{\sigma}_{\nu}, \tag{7.41}$$

which is usually interpreted as the equation of conservation of momentum and energy, when T^{ρ}_{ν} is identified as the energy–momentum tensor density. Consequently, in the presence of matter it is usual to modify the equations (7.28), thus:

$$R_{\lambda\mu} - \tfrac{1}{2}R^{\sigma}_{\sigma}g_{\lambda\mu} = -T_{\lambda\mu} - 2\kappa g_{\lambda\mu},$$

where $T_{\lambda\mu}$ is the energy–momentum tensor associated with the distribution of matter.

7.3.1 Classical Embedding of Schwarzschild's Solution

Here our primary aim will be to determine not the metric tensor $g_{\lambda\mu}$ but the vector ζ_{λ} in (7.40), from which the metric tensor is easily constructed. In its passage between its source and a point of observation, a particle traverses empty space and the form of Einstein's field equations that will be adopted is therefore $R_{\lambda\mu} = 3g_{\lambda\mu}/R^2$, as in (7.39), with the corresponding expressions obtained from (7.36) and (7.37) for the Riemannian and Ricci tensors. The simplest exact solution, first obtained by Schwarzschild, assumes that the metric tensor depends only on a radial coordinate r, identified with the distance from a central massive body such as the Sun. In the following we shall obtain this solution as a degenerate form of a somewhat more general solution which takes account of the cosmological term.

The distance r and the time t can both be assumed to be very small on a cosmological scale, so that the exact fulfillment of the normalization condition $\bar{\zeta}\zeta = 1$ is not mandatory, and instead the condition

$$\det(-g_{\lambda\mu}) = \det(-h_{\lambda\mu}) \tag{7.42}$$

is imposed, with the implication that $g_{00} \approx h_{00} = 1$.

At least six non-vanishing components $\zeta^{(j)}$ of the vector ζ are required, and may be defined by

$$\zeta^{(0)} = \mu f(r)\sinh(t/\mu), \qquad (\zeta^{(1)}, \zeta^{(2)}, \zeta^{(3)}) = r(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta),$$

$$\zeta^{(4)} = \mu f(r)\cosh(t/\mu), \qquad \zeta^{(5)} = h(r), \tag{7.43}$$

with the adoption of coordinates $x^{\lambda} = (t, r, \theta, \varphi)$, where t is the time and (θ, φ) are spherical polar angles. The interval is then given by

$$d\tau^2 = g_{\lambda\mu}dx^{\lambda}dx^{\mu} = \bar{\zeta}_{\lambda}\zeta_{\mu}dx^{\lambda}dx^{\mu} = f^2dt^2 - f^{-2}dr^2 - r^2(d\theta^2 + \sin^2\theta d\varphi^2),$$

$$f^{-2} = 1 + \mu^2 f'^2 + h'^2. \tag{7.44}$$

Of Einstein's field equations, that involving R_{00} is most easily evaluated. If we denote the time-dependent component $(\zeta^{(0)}, 0, 0, 0, \zeta^{(4)}, 0)$ of ζ by v we may write

$$\zeta_0 = v_0 = \epsilon v, \qquad \epsilon\eta = -\eta\epsilon, \qquad \epsilon^2 = -h_{00} \tag{7.45}$$

so that $g_{00} = \bar{v}v = f^2$ and

$$R_{00} = \bar{v}^{\nu}\epsilon v_{\rho}\bar{v}^{\rho}\epsilon v_{\nu} - \bar{v}^{\nu}_{,\nu}v = 0.$$

From (7.18),

$$(-g)^{\frac{1}{2}}\bar{v}^{\nu}_{/\nu} = ((-g)^{\frac{1}{2}}\bar{v}^{\nu})_{,\nu}, \qquad g = \det(-g_{\lambda\mu}), \tag{7.46}$$

so that this equation may also be written

$$R_{00} = (-g)^{-\frac{1}{2}}((-g)^{\frac{1}{2}}\bar{v}^{\nu}v)_{,\nu} + \bar{v}^{\nu}\epsilon v_{\rho}\bar{v}^{\rho}\epsilon v_{\nu} = 0. \tag{7.47}$$

Now

$$\bar{v}^{\nu}\epsilon v_{\rho}\bar{v}^{\rho}\epsilon v_{\nu} = \bar{v}^{0}\epsilon v_{\rho}\bar{v}^{\rho}\epsilon v_{0} + \bar{v}^{\nu}\epsilon v_{0}\bar{v}^{0}\epsilon v_{\nu}$$

$$= -2f^{-2}\bar{v}v_\rho\bar{v}^\rho v = -2f^{-2}ff_\rho(\bar{v}^\rho v)_{,\rho},$$

so we have

$$\tfrac{1}{2}\Box f^2 = -\kappa, \qquad \Box = \eta^{\lambda\mu}\partial_\lambda\partial_\mu,$$

where $\Box$ is D'Alembert's differential operator, with the solution,

$$f^2 = 1 - 2m/r - \tfrac{1}{3}\kappa r^2, \tag{7.48}$$

where m is a constant of integration. But for static solutions (with $\kappa = 0$) and spherical symmetry, this equation leads to the well known generalization of Schwarzschild's solution

$$f^2 = 1 - 2m/r - r^2/R^2 \qquad (g = -1),$$

$$d\tau^2 = f^2dt^2 - f^{-2}dr^2 - r^2(d\theta^2 + \sin^2\theta d\phi^2) \tag{7.49}$$

in spherical polar coordinates.

The zeros of the function f^2 correspond to horizons near the surface of the Schwarzschild sphere. There are corresponding singularities of the function f^{-2} which have been endowed with the somewhat fanciful names 'black hole' and 'big bang'. The latter is derived from cosmological models proposed by Robertson and Friedman, for which however vectors ζ can be constructed related to the vector defined in (7.43) by a suitable choice of the radial coordinate. It is worth noticing that both of singularities recede as they are approached. For general values of m and R, the condition $g = \det(\eta_{\lambda\mu})$ serves merely to define a coordinate r, but the geodesic distance σ_r between two points on a radius vector is given by

$$\frac{dr}{d\sigma_r} = f, \qquad \sigma_r = \int_{r'}^{r} dr/f, \tag{7.50}$$

where σ_r is the separation between two points in the r-direction, derived from $d\sigma^2 = -d\tau^2$ and the general definition of τ given in (7.49). But the singularities near $r = 2m$ and $r = R$ in the integral of (7.50) involve only inverse square roots and can both be removed by a change of variable involving hyperelliptic functions. They would not be apparent to an observer in the neighborhood of the singularities.

In the absence of the cosmological term we recover Schwarzschild's solution, and in this instance the function $h(r)$ in (7.43) and (7.44) can be evaluated in term of known functions. Neglecting κ, we choose $\mu = 4m$ in (7.43) so that the resulting equation for h becomes

$$h' = \mathrm{e}^{-2\rho}(\mathrm{e}^{2\rho} + 1 + \mathrm{e}^{-2\rho})^{\frac{1}{2}}, \qquad \mathrm{e}^{2\rho} = r/(2m)$$

so that

$$h = 2\mu\int(\mathrm{e}^{2\rho} + 1 + \mathrm{e}^{-2\rho})^{\frac{1}{2}}d\rho.$$

This integral can be evaluated in terms of elliptic functions of modulus $k = \frac{1}{2}$ and complementary modulus $k' = \frac{1}{2}\sqrt{3}$. If

$$\cosh\rho = \mathrm{dc}\,z, \qquad \sinh\rho = k'\mathrm{sc}\,z, \qquad d\rho = k'\mathrm{nc}\,zdz;$$

then

$$h = 4\mu k'^2\int \mathrm{nc}^2 zdz = 4\mu[-E(z) + k'^2 z + \mathrm{dn}\,z\mathrm{sc}z],$$

where $E(z)$ is the elliptic function of the second kind. When the cosmological constant is not neglected, h is a higher transcendental function.

7.3.2 More General Solutions of Einstein's Equations

If we substitute from (7.21), we obtain Einstein's equations (with the cosmological term) in the form

$$\bar{\zeta}^\nu_{/\nu}\zeta_{\lambda/\mu} - \bar{\zeta}^\nu_{/\mu}\zeta_{\lambda/\nu} = \kappa\bar{\zeta}_\lambda\zeta_\mu. \tag{7.51}$$

Again we choose coordinates such that $\det(g_{\lambda\mu}) = \det(h_{\lambda\mu})$, and then, by differentiating with respect to x^ν and making use of (A.20) and (7.17) we have

$$g^{\mu\lambda}g_{\lambda\mu,\nu} = \Gamma^\mu_{\mu\nu} = 0, \qquad \bar{\zeta}^\nu_\nu = 0. \tag{7.52}$$

In most known solutions, the metric tensor does not depend on one at least of the four coordinates, which we denote by x^τ, on the understanding that the summation convention for repeated greek affixes should not apply to τ. By a change of coordinates if necessary we can ensure that $g_{\nu\tau} = 0$ when $\nu \neq \tau$. Next we set $\lambda = \mu = \tau$ in (7.51) and write

$$\zeta_\tau = \xi_\tau = \sigma\xi, \qquad \bar{\zeta}_\tau = \bar{\xi}_\tau = -\bar{\xi}\sigma, \qquad \sigma^2 = -\eta_{\tau\tau}, \qquad \bar{\xi}\xi = f^2, \tag{7.53}$$

so that $g_{\tau\tau} = f^2\eta_{\tau\tau}$ and $g_{\lambda\mu,\tau} = 0$. Then this equation reduces to

$$\bar{\xi}^\nu\sigma z'\sigma\xi_\nu - \eta_{\tau\tau}\bar{\xi}^\nu_{,\nu}\xi = \kappa\eta_{\tau\tau}\bar{\xi}\xi,$$

i.e.,

$$(\bar{\xi}^\nu\xi)_{,\nu} + \eta_{\tau\tau}\bar{\xi}^\nu\sigma\xi_\rho\bar{\xi}^\rho\sigma\xi_\nu = -\kappa f^2. \tag{7.54}$$

Now as $g_{\nu\tau} = 0$ if $\nu \neq \tau$, $\bar{\zeta}^\rho\zeta_{\nu,\tau} = 0$ unless $\rho = \tau$ or $v = \tau$ (but not both). So

$$\bar{\xi}^\nu\sigma\xi_\rho\bar{\xi}^\rho\sigma\xi_\nu = \bar{\xi}^\tau\sigma\xi_\rho\bar{\xi}^\rho\sigma\xi_\tau + \bar{\xi}^\nu\sigma\xi_\tau\bar{\xi}^\tau\sigma\xi_\nu$$

$$= -2\eta_{\tau\tau}f^{-2}\bar{\xi}\xi_\rho\bar{\xi}^\rho\xi = -2\eta_{\tau\tau}f^{-2}ff_\rho(\bar{\xi}^\rho\xi)_{,\rho}$$

and the equation is, finally,

$$(f^{-2}\bar{\xi}^\nu\xi)_{,\nu} = -\kappa. \tag{7.55}$$

To obtain a generalization of the Schwarzschild solution, we note that only terms with $\nu \neq \tau$ survive, and if, to satisfy $\det(g^{\lambda\mu}) = -1$, we take $g^{\nu\rho} = f^2\eta^{\nu\rho}$ for $\nu \neq \tau$ and $\rho \neq \tau$, the equation reduces further. More generally, the metric tensor is

$$g_{\lambda\mu} = \eta_{\lambda\mu} + (f^2 - 1)\delta^\tau_\lambda \eta_{\tau\mu} + f_\lambda f_\mu + g_\lambda g_\mu, \tag{7.56}$$

and, again on account of the condition $\det(g_{\lambda\mu}) = -1$, g is related to f by the partial differential equation

$$\Delta \equiv (f)^2[(1 + \bar{f}^\lambda f_\lambda)(1 + \bar{g}\lambda g_\lambda) - (\bar{f}^\lambda g_\lambda)^2] = 1, \tag{7.57}$$

where $\bar{f}^\lambda = \eta^{\lambda\mu} f_\mu$ and $\bar{g}^\lambda = \eta^{\lambda\mu} g_\mu$. The contravariant components of f_λ and g_λ are

$$f^\lambda = \tfrac{1}{2}\,\partial\Delta/\partial f_\lambda = (f)^2[(1 + \bar{g}^\mu g_\mu)\bar{f}^\lambda - \bar{f}^\mu f_\mu \bar{g}^\lambda), \qquad g^\lambda = \tfrac{1}{2}\,\partial\Delta/\partial g_\lambda. \tag{7.58}$$

7.3.3 Lagrangian Densities

There are several Lagrangian densities from which the different forms we have given of Einstein's gravitational field equations can be derived. One is essentially the negative of the scalar curvature $R = R^\lambda{}_\lambda$, converted into a density $\mathcal{R}$ by multiplication with $(-g)^{\frac{1}{2}}$, but as this includes terms which involve the second derivatives of the metric tensor $g_{\lambda\mu}$, which is the fundamental field variable in this formulation, the Lagrangian density in the absence of the cosmological term is more conveniently defined as

$$\mathcal{L} = (-g)^{\frac{1}{2}} g^{\mu\nu}(\Gamma^\lambda_{\rho\mu}\Gamma^\rho_{\lambda\nu} - \Gamma^\lambda_{\lambda\rho}\Gamma^\rho_{\mu\nu}) = [(-g)^{\frac{1}{2}}(-g^{\mu\nu}\Gamma^\lambda_{\mu\nu} + g^{\mu\lambda}\Gamma^\nu_{\nu\mu})]_{,\lambda} - \mathcal{R},$$

$$\mathcal{R} = (-g)^{\frac{1}{2}} R = (-g)^{\frac{1}{2}} g^{\mu\nu}(-\Gamma^\lambda_{\mu\nu,\lambda} + \Gamma^\lambda_{\lambda\mu,\nu} + \Gamma^\lambda_{\rho\mu}\Gamma^\rho_{\lambda\nu} - \Gamma^\lambda_{\lambda\rho}\Gamma^\rho_{\mu\nu}),$$

with the Christoffel affinity expressed in terms of the metric tensor, as in (7.27). The expression given for $\mathcal{L}$ can be further simplified if $(-g)^{\frac{1}{2}} = (-h)^{\frac{1}{2}}$, since then $\Gamma^\lambda_{\lambda\rho} = 0$.

*The variation of this Lagrangian density with respect to the metric tensor is still not very simple, but yields the desired results.

However, in terms of the vectors ζ_λ and $\bar{\zeta}^\lambda$, no such compromise is necessary. The Lagrangian density is again essentially the negative of $\mathcal{R}$, but includes terms involving a matrix parameter κ, subsequently identified as a unit multiple of the cosmological constant:

$$\mathcal{L} = \bar{\zeta}^\lambda z^\dagger{}_\mu z^{\dagger\mu}\zeta_\lambda - \bar{\zeta}^\lambda z^\dagger_\lambda z^{\dagger\mu}\zeta_\mu - \bar{\zeta}^\lambda\kappa\zeta_\lambda) - \mathrm{tr}(\kappa z^\dagger + \kappa). \tag{7.59}$$

Variation of this Lagrangian density with respect to κ yields the required expression $z^\dagger = 1 - \zeta^\mu\bar{\zeta}_\mu$ for the projection $z^\dagger$, while variation with respect to ζ_λ yields the required field equation

$$R_{\lambda\mu} = \bar{\zeta}^\nu_{/\nu}\zeta_{\lambda/\mu} - \bar{\zeta}^\nu_{/\mu}\zeta_{\lambda/\nu} = \kappa\bar{\zeta}_\lambda\zeta_\mu.$$

Finally, the equations satisfied by the functions f and g appearing in (7.58), together with all other required relations can be derived from the Lagrangian density

$$\mathcal{L} = \alpha_\lambda f f^\lambda + 2\alpha f_\lambda f^\lambda + \beta_\lambda[f^\lambda/f - f(1 + \bar{g}^\mu g_\mu)\bar{f}^\lambda + f\bar{f}^\mu f_\mu \bar{g}^\lambda] + \gamma(\Delta - 1).$$

7.4 Quantal Embedding

In the introduction to this chapter we have suggested an interpretation of Einstein's gravitational and cosmological theories based on the definition of the metric tensor in (7.56) in terms of the relativistic density matrices of the neutral particles that provide the geometrical information. So far this could be considered equivalent to the embedding of the Riemannian space of the universe in the vector space of the spin matrices of the elementary particles. The possibility of the classical embedding of non-euclidean manifolds in both flat and curved manifolds has been known for a long time and has been exploited in the literature. However, we shall now adopt a different approach, corresponding to what could be called the *quantal* embedding of the Riemannian space, since the 'coordinates' of the embedding space are not the components of the vector ζ but parameters of the group of transformations connecting different vectors ζ_o and ζ. In this section we shall show how to determine these parameters, and obtain some explicit results, including remarkably simple results (in terms of elementary functions) for the Schwarzschild metric.

As foreshadowed in the discussion following (7.10), the vector ζ_s representing a neutral particle at its source is assumed to be in a representation of with highest weights $(s, s, \pm s)$. The vector may be assumed to be an eigenvector of the commuting matrices α_{03}, α_{12} and α_5 representing the selected observables which we have identified with the momentum, the spin and the helicity respectively:

$$\alpha_{03}\zeta_s = s\zeta_s, \qquad \alpha_{12}\zeta_s = s\zeta_s, \qquad \alpha_5\zeta_s = s\zeta_s. \tag{7.60}$$

Then, if as in (7.9) we denote the generators of $SO(4,2)$ in this representation by α_{jk} and α_l and these are expressed in terms of the irreducible representations of spin $\frac{1}{2}$, thus:

$$\alpha_{jk} = \sum_r \alpha^{(r)}_{jk}, \qquad \alpha_l = \sum_r \alpha^{(r)}_l, \tag{7.61}$$

the $\alpha^{(r)}_{jk}$ and $\alpha^{(r)}_l$ are in representations with highest weights $(\frac{1}{2}, \frac{1}{2}, \pm\frac{1}{2})$, and it follows that each of the spinor components $\alpha^{(r)}_{03}$, $\alpha^{(r)}_{12}$ or $\alpha^{(r)}_5$ obtained from

(7.61) has eigenvalues $\frac{1}{2}$, $\frac{1}{2}$ or $\pm\frac{1}{2}$ respectively on a highest weight vector of the representation:

$$\alpha_{03}^{(r)}\zeta_s = \tfrac{1}{2}\zeta_s, \qquad \alpha_{12}^{(r)}\zeta_s = \tfrac{1}{2}\zeta_s, \qquad \alpha_5^{(r)}\zeta_s = \pm\tfrac{1}{2}\zeta_s. \tag{7.62}$$

These equations completely determine the vector ζ_s, as a direct product of factors $\zeta_s^{(r)}$ for spin $\frac{1}{2}$, and also allow the vector ζ at any other point z of space-time to be expressed in terms of products of spinor factors:

$$\zeta_s = \prod_{r=1}^{2s}\zeta_s^{(r)}, \qquad \zeta = u\zeta_s = \prod_{r=1}^{2s}\zeta^{(r)}, \qquad \zeta^{(r)} = u^{(r)}\zeta_s^{(r)}, \tag{7.63}$$

where u and the $u^{(r)}$ are pseudo-orthogonal ($\bar{u} = \eta u^{\mathrm{t}}\eta = u^{-1}$) matrices connecting the points z_s and z. Now $g_{\lambda\mu} = \bar{\zeta}_\lambda\zeta_\mu$ where

$$\zeta_\lambda = \sum_r \zeta_\lambda^{(r)} \prod_{s\neq r}\zeta^{(s)},$$

and since $\bar{\zeta}_\lambda^{(r)}\zeta^{(r)} = 0$, it follows from (7.63) that

$$g_{\lambda\mu} = \sum_{r=1}^{2s}\bar{\zeta}_\lambda^{(r)}\zeta_\mu^{(r)} = \sum_{r=1}^{2s}\bar{\zeta}_s^{(r)}\bar{u}_\lambda^{(r)}u_\mu^{(r)}\zeta_s^{(r)}. \tag{7.64}$$

Each term under the summation corresponds to an irreducible representation of spin $\frac{1}{2}$, and also commutes with the other terms under the summation, so that *it will be sufficient for the purposes of this section to consider the irreducible representations for spin* $\frac{1}{2}$. But since the metric tensor is represented as the sum of $2s$ identical term, it is proportional to the spin. This spin dependence of the metric tensor can affect only the the apparent scale of the universe; however, it is possible that by the admittedly difficult comparison of of the time of transit of light and neutrinos between a source and a detector, this particular feature of the present interpretation of Einstein's theory may be tested experimentally in the future.

In the classical theory developed by Einstein, a particle moving freely under gravity moves along a path which is the join $(z - z_s)^2/\sigma^2$, where $\sigma^2 = -\tau^2 = \frac{1}{2}\mathrm{tr}(z - z_s)^2$ of the points z_s and z of emission and absorption; the trajectory is computable with the help of an explicit expression for the interval $d\tau$, obtained from the integration of the gravitational field equations. In the quantum theory essentially the same calculation yields the variation of the relativistic density matrix of the particle between source and detector, but still requires an explicit form of the metric tensor or the corresponding vector ζ. The most general expression that can be written down for u in (7.63) has 28 independent functions of position, clearly sufficient to reproduce any metric tensor, in fact with considerable redundancy which can be attributed to the existence of gauge transformations $u \to \bar{v}uv$ which leave

the metric tensor unchanged. In the following, we shall show in more detail how the observation of neutral particles can provide information on the nature of space-time, by identifying particular elements u of the group $SO(6,2)$ corresponding to the special types of metric tensor for empty space derived in the previous section; for this purpose it is sufficient to define elements of the type

$$u = \exp(2i\omega^j\gamma_j) = \tilde{q} + 2iq^j\gamma_j, \qquad (j = 0, \ldots 6) \tag{7.65}$$

where the γ_j form a set of Dirac matrices defined so that $\{\gamma_j, \gamma_k\} = \frac{1}{2}h_{jk}$, with $h_{00} = 1$ but $h_{jk} = -\delta_{jk}$ for $j, k > 0$. Since $(\omega^j\gamma_j)^2 = \omega^j\omega_j$, the ω^j, and $\tilde{q}$ and q^j, are related by

$$\tilde{q} = \cos\omega, \qquad q^j = \omega^j \sin\omega/\omega, \qquad \omega^2 = \omega^j\omega_j. \tag{7.66}$$

*The exponential function in (7.65) can also be resolved into factors representing elementary cosmological and gravitational effects, including rotations and boosts.

In units with $R = 1$, the parameters ω_0, ω_1 and ω_2 have the same significance as t, φ and θ in (7.44), and $\omega_3 = \sin^{-1}r$ is the angular distance from the point z_o, while ω_4, ω_5 and ω_5 are the parameters which determine the gravitational field. Because $\bar{u}_\lambda u_\mu + \bar{u}_\mu u_\lambda$ is a multiple of the unit matrix, the form of u given in (7.65) has the special feature that the metric tensor is independent of the vector ζ_s in (7.62) and the latter can be expressed simply as

$$g_{\lambda\mu} = \tfrac{1}{2}(\bar{u}_\lambda u_\mu + \bar{u}_\mu u_\lambda) = \tilde{q}_\lambda\tilde{q}_\mu + q_\lambda^j q_{j\mu} \qquad (\tilde{q}^2 + q^j q_j = 1). \tag{7.67}$$

It seems likely that the metric tensor of any solution of the gravitational field equations can be expressed in the above form. To obtain static solutions of the type considered in the last section it is sufficient to substitute

$$q^0 = \mu f\sinh(t/\mu), \quad q^1 = r\sin\theta\cos\varphi, \quad q^2 = r\sin\theta\sin\varphi, \quad q^3 = r\cos\theta$$

$$q^4 = \mu f\cosh(t/\mu), \quad q^5 = \chi\cos\omega, \quad q^6 = \chi\sin\omega, \quad \tilde{q} = (1 - r^2 - \mu^2 f^2 - \chi^2)^{\frac{1}{2}}.$$

Then the interval $d\tau$ is given by $d\tau^2 = d\tilde{q}d\tilde{q} + dq^j dq_j$, or

$$d\tau^2 = f^2dt^2 - dr^2 - \mu^2 df^2 - d\chi^2 - \chi^2 d\omega^2 + d\tilde{q}^2 - r^2(d\theta^2 + \sin^2\theta d\varphi^2), \tag{7.68}$$

where f, χ and ω may be independent functions of position in general. The parameters q^4, q^5 and q^6 are coordinates in a three-dimensional subspace of the embedding space and though the metric tensor is unaffected by rotations in this subspace, such rotations do affect the properties of neutral particles propagating in the gravitational field.

Finally, we assume spherical symmetry, so that f, χ and ω are functions of r, and the formula (7.68) for the interval reduces to

$$d\tau^2 = f^2dt^2 - (1 + \mu^2 f'^2 + \chi'^2 + \chi^2\omega'^2 - \tilde{q}'^2)dr^2 - r^2(d\theta^2 + \sin^2\theta d\varphi^2), \tag{7.69}$$

where, as usual, the primes denote differentiation with respect to r. Assuming the results given in (7.49),

$$f^2 = 1 - 2m/r - r^2, \qquad f^{-2} = 1 + \mu^2 f'^2 + \chi'^2 + \chi^2 \omega'^2 - \tilde{q}'^2$$

and the expression for $\tilde{q}$ is simplified by the choice

$$\chi^2 = 1 - r^2(1 - 1/R^2), \qquad \tilde{q}^2 = 2\mu^2 m/r$$

then the condition $\det(g_{\lambda\mu}) = -\det(h_{\lambda\mu})$ yields the angle ω as the quadrature

$$\omega = \int^r [(1 - f^2 - f^2 f'^2)/f^2 - \chi'^2 + \tilde{q}'^2]^{\frac{1}{2}} dr/\chi \tag{7.70}$$

wherein, as in the classical embedding, the choice $\mu \approx 4m$ removes the singularity on the Schwarzschild sphere. In the Schwarzschild limit ($r \ll 1$), $\tilde{q}'^2$ is negligible and ω can be evaluated in terms of elementary functions:

$$\omega = \tfrac{1}{4}(2\gamma + \sinh 2\gamma), \qquad \gamma = \sinh^{-1}(r/2m)^{\frac{1}{2}},$$

whereas as we have seen the corresponding classical embeddings are in terms of elliptic functions or higher traanscendental functions. The quantal embeddings also have the important advantage over their classical counterparts that they have a direct physical interpretation and their parameters are in principle observable. Finally, they provide immediate solutions of the generalization of the Dirac–Majorana and Maxwell equations which will be considered in the next section. We shall make use the fact that the metric tensor in (7.67) can be expressed in the form

$$g_{\lambda\mu} = h^j_\lambda h_{j\mu}, \qquad h^j_\lambda = q^j_\lambda + q^j \tilde{q}_\lambda/(1 + \tilde{q}), \tag{7.71}$$

where the heptad of vectors h^j_λ is then simply related to $\tilde{q}$ and the q^j in (7.67). But from (7.65) it can already be seen that the gravitational field has the effect of inducing rotations in the space of the γ_4, γ_5 and γ_6-matrices and hence transitions between different helicities and 'flavours', with 'mixing angles' depending on ω^4, ω^5 and ω^6 that increase approximately as the change of the square root of the distance in terms of the radius of the Schwarzschild sphere (~ 3 km for the Sun).

When, in the spinor representation, u is of the form shown in (7.65), the metric tensor, given by (7.67), is independent of the vector ζ_s representing the particle at its source. If a change is made of the coordinates $q^j \to q^j + q^j_s$ of the 7-dimensional space of the vector q^j , q^j_s can be chosen so that $u = u_s$ at the point z_s, defined as the source of a particle with a given spin and momentum that may be observed subsequently at some other point z of space-time. The new parameters $q^j + q^j_s$ are invariant under all coordinate transformations and are computable by a definite procedure from physical measurements; unlike the coordinates $(t, \mathbf{r})$, they may therefore be regarded as 'physical', and the q^λ as 'physical coordinates' with an observable source as the origin.

7.5 Gauge Theories with Gravitation

Early in the development of the general theory of relativity, generalizations were found, most of which were intended to achieve a unification of Einstein's theory with Maxwell's theory of electromagnetic phenomena. One of these was due to Weyl, and can be classfied as a gauge theory, restricted to real gauge transformations $g_{\lambda\mu} \to \lambda^2 g_{\lambda\mu}$ affecting the metric tensor. A generalization of more enduring interest was found by Einstein himself, and was called his 'unitary' theory, to distingish it from the largely unsuccessful 'unified' theory which followed it. The unitary theory introduced a tetrad of vectors h^α_λ ($\alpha = 0, 1, 2, 3$), in terms of which the metric tensor of general relativity could be defined by $g_{\lambda\mu} = h_{\alpha\beta} h^\alpha_\lambda h^\beta_\mu$, and corresponding metric tensor of special relativity by $h^{\alpha\beta} = g^{\lambda\mu} h^\alpha_\lambda h^\beta_\mu$. It was soon realized that general relativistic analogues γ_λ of the Dirac matrices γ^α of special relativity could be defined by $\gamma_\lambda = h^\alpha_\lambda \gamma_\alpha$, and that on this basis generalizations of Dirac's equation and other realtivistic equations, so that the unitary theory could be connected with important areas of particle physics.

The expression for the metric given in (7.71) in terms of a heptad of vectors is an obvious generalization of that provided by Einstein's unitary theory, but to build a connection with information theory in this section we shall obtain a generalization of the equation for the vector ζ that determines the evolution of the relativistic matrix z of a neutral particle with its source at the point $z_s = \zeta_s \bar{\zeta}_s$. As discussed earlier, in order that information should be gained concerning this particle, it is usually necessary that it should be detected by an absorber at some point $z = \zeta\bar{\zeta}$, identified with the relativistic density matrix of the particle in some representation of $SO(5, 2)$. As in special relativistic theory, the vector ζ is regarded as some component of a quantized field variable ψ, which satisfies the same equation.

To obtain a generalization valid for arbitrary spin and invariant under all coordinate transformation, the Majorana–Kemmer matrices α_λ in (7.7) are replaced by

$$e_\lambda = \alpha_j h^j_\lambda \qquad (\lambda = 0, 1, 2, 3).$$

For any spin it follows from (7.9) and (7.71) that that these matrices satisfy

$$[e_{\lambda\mu}, e_\nu] = g_{\mu\nu} e_\lambda - g_{\lambda\nu} e_\mu, \qquad e_{\lambda\mu} = [e_\lambda, e_\mu],$$

so that the $e_{\lambda\mu}$ and e_ν are generators of a representation of $SO(3, 2)$ and are general relativistic analogues of the $\alpha_{\lambda\mu}$ and α_ν.

The matrices $e_{\lambda\mu}$ and e_ν in the above relations are not unique: if w is any pseudo-orthogonal matrix, $\bar{w} e_{\lambda\mu} w$ and $\bar{w} e_\nu w$ satisfy the same commutation relations; in particular, with the choice $w = u^{\frac{1}{2}}$, they are satisfied by $\tilde{e}_\lambda = i u_\lambda \bar{u}$ and $\tilde{e}_{\lambda\mu} = [\tilde{e}_\mu, \tilde{e}_\lambda]$. By writing

$$e_l = \alpha_j h^j_l, \qquad e_{lm} = \alpha_{jk} h^j_l h^k, \tag{7.72}$$

it is easy to verify that

$$[e_{lm}, e_p] = g_{mp}e_l - g_{lp}e_m, \qquad e_{lm} = [e_l, e_m], \tag{7.73}$$

in which it possible to restrict e_l to a pentad, hexad or heptad of matrices, all of which have found uses in the literature. There are also coordinate transformations that reduce $g_{\mu\nu}$ reduces to $\eta_{\mu\nu}$ at a particular point, e.g., at the source z_s of a particle, and the relations (7.73) then reduce at that point to the special relativistic form given in (7.9).

It is important to notice that, as a consequence of (7.34) and (7.35), the vector ζ must satisfy

$$\zeta^{\mu}_{/\mu/\nu} - \zeta^{\mu}_{/\nu/\mu} = 3\zeta_{\nu},$$

in units with $R = 1$, and, according to (7.31), this can be expressed in the algebraic form

$$[z^{\dagger}_{\nu}, z^{\dagger}_{\mu}]\zeta^{\mu} = 3\zeta_{\nu}, \tag{7.74}$$

equivalent to Einstein's equations with a cosmological term. The analysis of the last section has shown that these equations are satisfied by $\zeta = u\zeta_s$, with u given by (7.65). It is thus a important consequence of the present approach that for any initial value ζ_s *the solution* ζ *is already determined by Einstein's equations*, apart from a gauge transformation which leaves the metric tensor unchanged. As shown by (7.60), the vector ζ_s at the source of a particle carrying information is completely determined by the condition that ζ_s is an irreducible representation, labelled $(s, s, \pm s)$ of the representation of $SO(4, 2)$ for spin s.

There is a relatively simple transformation which allows the construction of the vector ζ_o at any point z_o on the trajectory of a particle travelling any direction from its source. For a particle of zero rest mass this is no more than a simple Lorentz transformation: it follows from (7.60) and

$$\alpha_{03}(\alpha_0 - \alpha_3) = (\alpha_0 - \alpha_3)(\alpha_{03} + 1)$$

that α_{03} has no eigenvalue $(s+1)$, and it follows that $(\alpha_0 - \alpha_3)\zeta_o = 0$, which can be interpreted as the equation of a particle of zero rest mass propagating in the x_3- direction. For a particle of non-vanishing mass m propagating in the same direction, a further transformation of the type

$$\zeta_s = u_s\zeta_o, \qquad u_s = \exp(w\alpha_{34})\exp(\omega\alpha_{04}), \qquad \cosh w = \operatorname{cosec}\omega = p_0/\mu,$$

corresponds to a translation to z_s from a point z_o on the cosmological or Schwarzschild horizon.

Analogues of the special relativistic equation (7.5) consistent with Einstein's equations, and therefore satisfied by ζ, are well known. The most general form can be written

$$\mathrm{i}e^{\lambda}(\zeta_\lambda - \Gamma_\lambda\zeta) = 0, \tag{7.75}$$

where Γ_λ depends on the gauge as well as position, and is invariant under pseudo-orthogonal transformations of the type

$$\zeta \to w\zeta, \qquad e^{\lambda} \to we^{\lambda}\bar{w}, \qquad \Gamma_\lambda \to w\Gamma_\lambda\bar{w} + w_\lambda\bar{w}. \tag{7.76}$$

Thus with $\Gamma_\lambda = u_\lambda\bar{u}$ the choice $w = \bar{u}$, with u given by (7.65), effects the transformation $\zeta \to \zeta_o$.

7.6 Summary

Gauge transformations which leave the metric tensor unchanged, are also of this type, and it is accepted today that such transformations are physically significant. For photons, gauge transformations are generally considered to be related to a strongly broken symmetry. But for spin $\frac{1}{2}$ transformations affecting the parameters q^4, q^5 and q^6 in (7.65) could have a simpler interpretation. Though the differences between neutrinos with different 'flavours' (β-, μ- and τ-neutrinos) are not yet fully understood, the concept of a gauge group connecting them is generally accepted.

In the present chapter we have presented a synthesis of general relativity and quantum mechanics, based essentially on information theory. The most striking outcome of the analysis is that the relativistic statistical matrix of a neutral particle may be viewed as a microcosm of the observable parts of space-time through which the particle may be transmitted. The geometrical properties, including cosmological and gravitational effects, are reflected in the variation with the space-time coordinates of the parameters of the orthogonal group of transformations of the quantal wave equations. These conclusions are to a large extent independent of the representations of $SO(6, 2)$ which have been assumed for the quantal embedding of the Riemannian manifold of general relativity. But there are also some interesting features that depend on the representation and on the wave equation assumed for the neutrinos. The geometry of the physical world has been found to depend at least in scale on the spin of the particles by means of which the universe is observed, and there are gauge groups associated with the wave equation which are independent of, but are closely associated with the Riemannian metric of general relativity, and could provide new insights into properties of neutral particles.

8. Measurement and the Observer

The ultimate recipient of information of any kind is the conscious observer, and it is remarkable that although the anatomy and physiology of the animal brain have been extensively investigated since the time of Ramon y Cajal, its unique role in the processing of information was for a long time poorly understood and was one of the last applications of physics and information theory to have received attention. A role for quantum mechanics in the functioning of the brain was suggested to some physicists like Bohr and neurophysiologists like Eccles, perhaps influenced by a conviction that voluntary action was not predetermined, but also supported by evidence that at least visual sensory perception could be elicited by just a few photons. But for many years a credible mechanism for more general manifestations of quantum mechanical effects in the animal brain was lacking, in retrospect because such effects were believed to be associated with anatomical structures instead of the electrochemical activity of the cortex. In order to understand the phenomena of consciousness it would be necessary to take account of the role of fluctuating potentials in the electrolytic environment of the cells which make up the cortex, and the means of transfer of information between this environment and the intracellular fluid, through sub-microscopic channels in the cellular membrane.

But in this chapter we shall begin with a rather general study of how microscopic or sub-microscopic phenomena can result in observable macroscopic effects, and the creation of new information, within a theory of observation initiated by the author and developed in the present context in association with Triffet, who is responsible for much of the material presented very concisely in Sects. 8.4–8.6 below. The theory of observation is an important component of a physically based account of the way information is assimilated and is created by the mind of the observer.

The application of information theory to the animal brain, however, requires a general understanding of phenomena at four different levels:

(1) At the *microscopic* level it is necessary to identify the nature of the crucial quantal events, which will be shown to occur in the electrochemical processing of information by the cellular membrane.

(2) At the *cellular* level it is important to understand the mechanism by which the quantal effects are amplified and reach macroscopic proportions in

the form of quite small and much larger fluctuations of electrical potential. The small fluctuations within cells, with an amplitude of a few mV, are known as *graded potentials*, while the larger fluctuations, with an amplitude of the order of 100 mV, are known as *action potentials*. The cells displaying action potentials are called *neurons*, but there are also cells, known as *glial cells*, which do not communicate directly with other cells but play a role in the overall electrochemical activity. The neurons are characterized as either excitatory or inhibitory, depending on their effect on other neurons at the *synapses*, where different neurons come into close proximity. Together, the neurons and glial cells occupy most of the animal cortex.

(3) At the level of the groups of closely associated neurons called *columns* or *zones*, which extend from near the surface into the other functional layers of the cortex, it has been found experimentally that excitatory and inhibitory cells are both represented in every unit column so as to provide delicately balanced synaptic inputs to the pyramidal and Purkinje cells, which are in turn responsible for the principal synaptic outputs of the cortex.

(4) At the level of the principal subdivisions of the cortex and their interconnections, experimental work has also revealed the essential functions of each subdivision, and its contribution to the overall activity of the brain. By considering these levels separately, it is possible to reduce the mode of operation of what could at first appear to be a very complex informational processing system to a few rather simple principles. We shall find that these principles are in some essential respects similar to those of the various artificial devices which have been invented for the study of sub-microscopic phenomena, but also have some additional characteristic features which are necessary for conscious behaviour.

The prospects of creating artificial consciousness are closely linked with the development of quantum computation, and one obvious approach to both endeavours is to imitate selectively natural features of the animal brain. But earlier chapters of this book have shown that in principle the invention of machinery for quantum computation could be inspired by almost every area of modern physics. To successfully replicate, or even to simulate consciousness, it is obviously essential to know in precise physical and informational terms what is meant by consciousness and how it operates. We shall find that there is a sense in which various conscious attributes, and especially the attribute of unpredictability, are exhibited in many natural phenomena, and we shall conclude this chapter with some reflections on this theme.

From the present point of view, one of the important features of the cortex is its ability to take notice of some small part of the continual stream of information brought to it by the senses. In this respect it functions in a similar way to artificial detectors of submicroscopic events.

8.1 Detectors and Measuring Devices

The macroscopic manifestation of an event originating at the sub-microscopic level may occur spontaneously under suitable conditions in nature, but also in a variety of devices developed for the detection of quantal events for experimental purposes under controlled conditions. The man-made devices include counters for the detection of particles emitted in radioactive decay, present in the cosmic radiation or extracted from accelerators and plasma machines, but much more detailed information is obtained from ionization and other chambers designed to reveal the track of any particle detected, and from the observation of the coincident or anti-coincident functioning of independent devices or components of the same device.

The common feature of all such devices is that they allow the single or multiple interaction of a particle with a macroscopic and therefore observable system under conditions where the state of the macroscopic system is palpably and irreversibly changed as a result of the interaction. The irreversibility of the process implies an increase in entropy, equivalent to a loss of information which is normally much larger than the information gained concerning the quantal event. The sensitivity of an effective device is of crucial importance, and in practice is secured by *the preparation of its interactive material in a physically, chemically or electrically metastable state.* It is the observable transition between this metastable state and a more stable state that conveys the essential information concerning the sub-microscopic event which would otherwise be undetected. These rather obvious prerequisites for the effective observation of quantal phenomena must be taken into account in any adequate theory of measurement. Specifically, the functional material of the detector must be macroscopic and in a metastable state which allows the quantal interaction to become manifest at the macroscopic level. The general quantum theory of the action of effective measuring devices to be presented in this section is designed to satisfy these exacting requirements. Later in this chapter we shall confirm that natural processes in the animal cortex display similar features, and result in the acquisition and creation of new information, which is subjective in the sense that it affects only one animal but objective in the sense that it results in macroscopic changes which *in principle* may be observed by anyone else.

In the light of information theory, it is clear that the result of the measurement of fundamental quantal observables such as energy, momentum and angular momentum can never be known with certainty in advance. Every system in nature is either in interaction with its environment or has been in interaction in the past, and information concerning such observables is lost in the process. Even if information to be gained from the immediate environment were taken into account, the uncertainty concerning this larger system would remain, and the information to be gained from the entire universe is impossible even to estimate. *It follows that the assumption, commonly made in the quantum mechanical literature, that the existing state of a system in*

nature is pure, in the sense that it can be represented by a single wave function or state vector, is an idealization that cannot be sustained. As to be expected, however, there are considerations that validate correct inferences based on an incorrect hypothesis. The most important of these is that *after* an ideal measurement has been made, and the result has entered the consciousness of an observer, it may be possible for the observer to infer that the system was in a pure state. Also, in a controlled experimental environment, the result of the measurement of an observable such as the spin of an elementary particle, may well be predictable. If it is predictable, the observable is what we have called a selected observable, and commutes with the statistical matrix.

The distinction between selected and unselected observables has important implications for the theory of measurement, and helps to resolve certain paradoxes that troubled de Broglie and other distinguished physicists conditioned by the wave mechanical formulation of quantum mechanics. De Broglie's paradox concerns a particle in a box in Paris, which is divided into two parts by the insertion of a impermeable partition. One part is sent to Tokyo, and an experiment is conducted there to determine whether the particle is in that part. At the instant when the result of the experiment is known, it also becomes known whether the part of the box remaining in Paris contains the particle or not. If the idea is entertained that the particle could be represented by a wave function, distributed between the two parts of the box, it would appear that some form of action at a distance must be assumed to accompany the process of observation! For the resolution of de Broglie's paradox, it must first be understood that the number of particles in an impermeable box is a selected observable, and that selected microscopic observables are not in an essentially different category from ordinary macroscopic observables. If the particle were a macroscopic object, the possibility of action at a distance at the instant of its perception would hardly be worthy of consideration. But apart from this, common sense suggests that the content of each part of a subdivided box is decided at the time when the subdivision is made.

*In fact the entropy associated with a set of particles in a box is proportional to the volume of the box but decreases as the logarithm of the particle density, so that at the time when an impermeable partition is inserted there is a decrease in the information to be gained .

Quite generally, following the development of information theory and a detailed theory of measurement, it has become clear that in principle the process of measurement of a selected observable does not result in a gain of information, but that wherever unselected observables are observed *quantum mechanics implies the discovery of new information in the process of measurement and observation.* In the literature various inequalities are proved which might seem to establish the opposite. In any macroscopic system manifesting irreversible processes such as viscosity, thermal conduction, diffusion, or chemical or nuclear reactions, the information to be gained concerning the

microscopic state of the system increases because of loss of information to its environment. It was already a consequence of the second law of classical thermodynamics that the entropy associated with a closed system could not decrease, and because of the equivalence of entropy with information to be gained, it would follow that the information to be gained concerning an observational system could never increase. However, this does not exclude the possibility of a gain of information concerning a subsystem forming a part of such a system, as a result of its interaction with other parts; moreover, as we shall show, there may be actual creation or discovery of new information concerning an observable of the subsystem, in the spite of the increase of entropy of the observational system as a whole. We shall demonstrate the dependence of this result on a subtle inequality of quantal information theory.

We begin by summarizing the essentials of the matrix formulation of quantum mechanics in the context of quantal information theory. As in (1.13) and (1.14), an observable a is represented by a matrix $\sum a_r g_r$, where the a_r are possible results of the measurement of the observable, and the g_r form a complete set of minimal idempotent matrices or projections:

$$g_r g_s = g_s \delta_{rs}, \qquad \sum_r g_r = 1, \qquad \mathrm{tr}(g_r) = 1, \tag{8.1}$$

For reasons given in Sect. 1.4, the g_r are also required to be hermitean. Where there is a continuum of possible results of a measurement, summations like $\sum_r$ in the above are interpreted as integrations $\int dr$. The measured values a_r are eigenvalues of the matrix a, and are most efficiently obtained by the factorization method given in Sect. A.4, which uses only the fact that the product of a matrix with its hermitean conjugate is positive definite.

In the absence of complete information, the state of the system must be represented by a statistical matrix P which is also hermitean, is positive definite, and satisfies

$$\mathrm{tr}(P) = 1. \tag{8.2}$$

To summarize the generally accepted interpretation of quantum mechanics, if $a = \sum a_r g_r$ is any observable, the probability that a measurement of a will yield the value a_r is

$$p_r = \mathrm{tr}(g_r P). \tag{8.3}$$

Because P is hermitean and positive definite, and the g_r are hermitean, the probabilities $\mathrm{tr}(g_r P) = \mathrm{tr}(g_r P g_r)$ thus defined are necessarily non-negative and the condition (8.2) reduces to $\sum p_r = 1$. The expectation value of a is

$$\langle a \rangle = \sum a_r p_r = \mathrm{tr}(aP). \tag{8.4}$$

The information to be gained from the measurement, regarded as an observable, is represented by the matrix

$$I = -\sum \log(p_r) g_r \tag{8.5}$$

and the expectation value of I is

$$\langle I\rangle = \mathrm{tr}(IP) = -\sum \log(p_r)p_r, \tag{8.6}$$

in agreement with Shannon's classical definition.

Now a *selected* observable is one that commutes with the statistical matrix, such as the energy of an isolated system in a stationary state, or the number of particles of a particular kind within an impermeable container as in de Broglie' paradox. If $\tilde{a} = \sum \tilde{a}_s\tilde{g}_s$ is a selected observable, then P can be expressed in the form

$$P = \sum \tilde{p}_s\tilde{g}_s, \tag{8.7}$$

where $\tilde{p}_s$ is the probability that a measurement of $\tilde{a}$ will yield the value $\tilde{a}_s$. The information gained by the measurement of the selected observable is not essentially different from that gained from the observation of a macroscopic event, where it is not usually regarded as created or discovered by the act of observation. However, from (8.3) and (8.7) we find that the probability that the measurement of a (which is not necessarily a selected observable) yields the value a_r is

$$p_r = \sum p_{rs}\tilde{p}_s, \qquad p_{rs} = \mathrm{tr}(g_r\tilde{g}_s). \tag{8.8}$$

The p_{rs} satisfy

$$\sum_r p_{rs} = \mathrm{tr}(\tilde{g}_s) = 1, \tag{8.9}$$

and reduce to δ_{rs} when a is the same as $\tilde{a}$. Since $p_{rs} = \mathrm{tr}(g_r\tilde{g}_s\tilde{g}_sg_r)$, where $\tilde{g}_sg_r$ is the hermitean conjugate of $g_r\tilde{g}_s$, it is always positive and may be interpreted as the conditional probability of observing the value a_r of a, *if* the value of the selected observable $\tilde{a}$ is $\tilde{a}_s$. We note that

$$p_{rr} = 1 - \sum_{s\neq r} p_{rs}, \qquad p_r = \tilde{p}_r + \sum_s p_{rs}(\tilde{p}_s - \tilde{p}_r).$$

The information to be gained from the measurement of the selected observable is

$$\tilde{I} = -\sum \log(\tilde{p}_r)\tilde{g}_r = -\log P, \tag{8.10}$$

with the expectation value

$$\langle\tilde{I}\rangle = -\sum \log(\tilde{p}_r)\tilde{p}_r = -\mathrm{tr}(P\log P). \tag{8.11}$$

This may be called the selected information, and in the literature it has been frequently used to determine the maximum information to be gained from a system. But, as we have already observed, it is not different in kind from the information to be gained from a macroscopic measurement; *it is, in principle, predictable*. On the other hand, the difference

$$\delta I = \langle I - \tilde{I}\rangle \tag{8.12}$$

may be regarded as the information created or discovered in the measurement of the observable a; *this is, in principle, unpredictable*. We shall show that it is always non-negative, so that the selected information is by no means the maximum to be gained.

We consider the effect on the value of $\langle I\rangle$, computed from (8.6) and (8.8), of small variations δp_{rr}, δp_{rs}, δp_{sr} and δp_{ss} in p_{rr}, p_{rs}, p_{sr} and p_{ss}, with $r \neq s$; for the conservation of probability such variations must be subject to the conditions

$$\delta p_{rr} = -\delta p_{rs} = -\delta p_{sr} = \delta p_{ss} \tag{8.13}$$

so that the consequent change in $\langle I\rangle$ is

$$\begin{aligned}\delta I &= [(1+\log p_r)((\tilde{p}_r - \tilde{p}_s)\delta p_{rs} + (1+\log p_s)((\tilde{p}_s - \tilde{p}_r)\delta p_{sr}\\ &= \sum_{r,s}(\tilde{p}_r - \tilde{p}_s)\log(p_r/p_s)\delta p_{rs}.\end{aligned} \tag{8.14}$$

If the variations are from the 'selected' values $\tilde{p}_r$, the coefficients of the δp_{rs} are $(\tilde{p}_r - \tilde{p}_s)\log(\tilde{p}_r/\tilde{p}_s)$ and are always non-negative and, as $\delta p_{rs} = p_{rs} \geq 0$, δI is non-negative and is zero only if $\tilde{p}_r = \tilde{p}_s$. Thus $\langle I\rangle$ has a minimum when $p_{rs} = 0$.

More generally, since

$$\frac{\partial\langle I\rangle}{\partial p_{rs}} = (\tilde{p}_r - \tilde{p}_s)\log(p_r/p_s), \qquad \frac{\partial^2\langle I\rangle}{\partial p_{rs}^2} = -(\tilde{p}_r - \tilde{p}_s)^2(1/p_r + 1/p_s), \tag{8.15}$$

the only other extrema of $\langle I\rangle$ occur when $p_r = p_s$, and are maxima. The absolute maximum of $\langle I\rangle$ occurs when all the p_t are equal, so that nothing is known about the value of a. This is what we wished to prove.

The result is to enable a distinction to be made between quantal information that is not different in principle from classical information and information that represents a new discovery. We are able to conclude, on the basis of quantum mechanics, that the creation of new information is possible, and have obtained a general expression from which it can be calculated. We shall next obtain some even more fundamental results relevant to the theory of measurement.

8.1.1 Theory of Measurement

Physics, and the natural sciences in general, are concerned with the collection of empirical information concerning the world of common perception, and the condensation of this information into rules or 'laws', which can then be used

for the purpose of reliable prediction. In the past the study of planetary motion provided a good example. But since the discovery of quantum mechanics it has become clear that, especially for certain phenomena at the submicroscopic level, there is no known basis for definite prediction. For this reason Einstein regarded quantum mechanics as an incomplete theory which was sufficient only for statistical purposes. There are several newly developed or developing applications of quantum mechanics, however, in particular quantum computing, physically based theories of consciousness and the quantum theory of measurement that require more than statistical validity.

The possibility of quantum computation has attracted widespread attention from computer scientists and physicists in recent years. Originally suggested by Benioff , and explored in some detail by Deutsch and Josza, the interest in this prospect has been heightened by the realization that quantum processors might be very much more efficient in certain types of computation than their classical counterparts, because of their capacity for 'quantum parallelism'. In principle, an *unlimited* amount of information could be obtained from a single measurement by such a processor; however, some difficulty might well arise in both the selection and detection of the information. As should be clear from earlier chapters of this book, the elementary qubits on which a quantum computer might operate are components of common observables of physics, of which the spin angular momentum of a microscopic system is only one example. The practical problems of 'writing' and 'scanning' individual components in an extended sequence of qubits of this kind are quite formidable, especially if the results of these operations are required to be reproducible and therefore predictable in principle. In Chap. 2 we have emphasised the importance of the groups of similarity transformations, which in the context of quantum computing would be required to convert an observable to selected form in which the eigenvalue realized by measurement is in fact predictable in principle. In contrast, in a theory of consciousness such as will be developed later in this chapter, the application of quantum mechanics to individual events in the animal brain is expected to have an essentially unpredictable though highly correlated outcome.

In the following, our immediate aim will be to investigate in general terms the conditions under which applications of quantum theory requiring more than statistical validity may be validated. The results will also serve to clarify questions in the theory of measurement which were for many years an area of contention between theoretical physicists of great distinction.

Let us consider the interaction of a microsystem S′ with a detector S″ in the interaction representation. The statistical matrix P_0 of the joint system at a time $t = 0$ before the interaction is a direct product $P'_0 \otimes P''_0$ of the statistical matrices of the subsystems, so that for time t

$$P = T(P'_0 \otimes P''_0)\overline{T}, \tag{8.16}$$

where T is unitary and reduces to 1 at time $t = 0$.

The important problem is to show that soon after the interaction, under certain conditions, and for all practical purposes, P *consists of two parts, one corresponding to the possibility that the detector* S″ *functioned, and the other to the possibility that it did not.* Thus, although T is unitary, if the interaction results in the measurement of an unselected observable, what is called the coherence in the initial state of S' is effectively destroyed. We again emphasise that, for the solution of this problem it is necessary to suppose

(1) that the detector is macroscopic, consisting of a huge number of microsystems

(2) that the detector is efficient, implying that it is in a metastable state and the interaction with the microsystem, if it occurs, is easily detected by a transition to a more stable state, with a macroscopically significant increase of entropy (or, equivalently, a large loss of microscopic information concerning the detector).

We note first the T-matrix is unitary and therefore can be written in the form

$$T = \sum_{r+} g_{r+} \otimes T_{r+} + \sum_{r-} g_{r-} \otimes 1, \tag{8.17}$$

where the T_{r+} are unitary and g_{r+} and g_{r-} are idempotents of the observable a' of S′ measured by the detector; the latter are unaffected by the interaction and correspond to those values of a' for which the detector does not function. If the observable is selected, the g_{r+} and g_{r-} are all orthogonal: $g_{r+}g_{r-} = 0$, and no new information can be created or discovered. But where the observable is unselected, the substitution of (8.17) in (8.16) yields a sum of four terms:

$$P = TP_0\overline{T} = P_{++} + P_{+-} + P_{-+} + P_{--}, \tag{8.18}$$

all of which have a non-vanishing trace. The statistical matrix of the microsystem is obtained by taking a trace of the matrix factors associated with the detector, thus:

$$P' = P'_{++} + P'_{+-} + P'_{-+} + P'_{--}, \qquad P'_{++} = \sum_{r+,s+} \mathrm{tr}''(T_{r+}P''_0\overline{T}_{s+})g_{r+}P'_0g_{s+},$$

$$P'_{+-} = \sum_{r+,s-} \mathrm{tr}''(T_{r+}P''_0)g_{r+}P'_0g_{s-}, \qquad P'_{--} = \sum_{r-,s-} g_{r-}P'_0g_{s-}.$$

The statistical matrix of the detector, on the other hand, is obtained by taking a trace of the factor associated with the microsystem; as should be expected of a macroscopic object, it consists exclusively of terms corresponding to the possibility that the detector functioned, or did not function:

$$P'' = P''_+ + P''_-, \qquad P''_+ = \sum_{r+} p'_{r+}(T_{r+}P''_0\overline{T}_{r+}), \qquad p'_{r+} = \mathrm{tr}'(g_{r+}P'_0),$$

$$P''_- = (1-p'_+)P''_0, \qquad p'_+ = \sum_{r+} p'_{r+} = \sum_v p'_{r,v}p_v, \qquad p'_{+,v} = \mathrm{tr}'(\sum_{r+} g_{r+}g_v), \tag{8.19}$$

where p'_+ is the probability that the measurement of a' should yield the value a'_+ and $p'_{+,v}$ is the probability of a transition between the initial state g_v, of the microsystem and g_{r+}. The problem which we have undertaken is to show that C_{r+} in

$$P'_{+-} = \sum_{r^+,s^+} C_{r+}(g_{r+}P'_0 g_{s-}), \qquad C_{r+} = \mathrm{tr}''(T_{r+}P''_0) \tag{8.20}$$

tends to a value indistinguishable from zero as a result of the interaction. Write

$$P''_0 = \sum_{s_1} p^*_{s_1} g^*_{1,s_1} P_{s_1}, \qquad P_{s_1\ldots s_{m-1}} = \sum_{s_m} p^*_{s_1\ldots s_m} g^*_{m,s_m} P_{s_1\ldots s_m},$$

$$T_{r+} = \sum_{r_1} t_{r_1} g_{1,r_1} T_{r_1}, \qquad T_{r_1\ldots r_{m-1}} = \sum_{r_m} t_{r_1\ldots r_m} g_{m,r_m} T_{r_1\ldots r_m}, \tag{8.21}$$

where $|t_{r_1\ldots r_m}| = 1$, so that $T_{r_1\ldots r_m}$ is unitary and varies with the time.

If the detector functions, its change in entropy or information is determined by the matrix

$$T_{r+}P''_0\overline{T}_{r+} = \prod_{r_m}\sum_{s_1\ldots s_m} p^*_{s_1..s_m}(g_{m,r_1..r_m}g^*_{m,s_1..s_m}g_{m,r_1..r_m}), \tag{8.22}$$

so that a macroscopic change in entropy requires a significant change in a very large number of transition probabilities $\mathrm{tr}(g_{m,r_1..r_m}g^*_{m,s_1..s_m})$. But according to (8.20),

$$C_{r+} = \prod_{r_m}\sum_{s_1..s_m} t_{r_1..r_m}p^*_{s_1..s_m}\mathrm{tr}(g_{m,r_1..r_m}g^*_{m,s_1..s_m}), \tag{8.23}$$

and this is clearly a product of expectation values of the complex factors $t_{r_1..r_m}$ of modulus unity. Initially, $T_{r+} = 1$, and $g_{m,r_m} = g^*_{m,r_m}$, so that the factors $t_{r_1..r_m}$ all reduce to 1; but when the stated conditions are met, very many of them must rapidly deviate appreciably from unity. *Since the modulus of the expectation value of a set of complex numbers of unit modulus but different from unity is less than unity,* C_{r+} is exhibited as the product of a huge number of factors of modulus appreciably less than unity, and is therefore not rigorously zero but indistinguishable from zero. There is, therefore, effectively complete decoherence of the initial superposition of observable eigenstates of the microsystem.

The above is a much generalized form of an argument given originally by the author, where the detector was modelled by a set of coupled oscillators in a metastable state. The argument also shows that new information is discovered

in the process of measurement, unless the component P'_{+-} of P in (8.20) is rigorously zero, when the result of the measurement (as in de Broglie's paradox) is selected and, in principle, predictable in advance. This would be highly desirable in devices intended for quantum computation, though not in the functioning of the conscious brain. With the latter application in mind shall now proceed to a concise discussion of various subjects relevant to the phenomenon of consciousness.

8.2 Qubits of Fluctuating Electrolytic Potentials

In the nervous system of an animal, both the extracellular and intracellular transmission of information are through electrolytic media. We shall introduce our discussion of significant activity at the microscopic level with a brief account of the ionic composition of these media. The theory of electrolytes is in many respects similar to the theory of ionized gases, but there are differences arising from the abundance of water molecules in an aqueous electrolyte. Water is a polar liquid, whose molecules have well defined centres of positive and negative charge, resulting from a degree of separation of the H^+ and OH^- ions which make up each molecule. The presence of a positively charged (metallic) ion in solution results not only in the attraction of OH^- ions of neighbouring water molecules to the charge, but further polarizes those molecules, which then form a roughly spherical shell of hydration with a resultant negative charge around the positive ion. Similarly a negatively charged (basic) ion attracts H^+ ions belonging to neighbouring water molecules which then form a hydration shell with a resultant positive charge around the negative ion. Some of the different types of hydrated ions, the most important of which in the context of applications to the animal cortex are potassium, sodium, calcium, and chloride (K^+, Na^+, Ca^{++} and Cl^-) are listed below, together with estimates of their size and hydration numbers, i.e., the mean numbers of water molecules in their hydration shells.

Type of ion	K^+	Na^+	Ca^{++}	Cl^-
Mean radius (10^{-8} cm)	1.33	0.95	0.99	1.81
Hydration number	4	5	12	1

Electrolytes may be subjected to electrolysis, in which an electric current is generated by the diffusion of ions towards oppositely charged electrodes immersed in the solution. But this has little relevance in the biological context, where the energy of electric currents, both within and near the surface of cells, is derived ultimately from metabolic activity but more directly from a difference of electric potential between the interior of the cells and their immediate environment. The ionic concentrations of the extracellular fluid are rather similar to those of sea water, perhaps indicative of the origins of life, with an excess of sodium over potassium. On the other hand, metabolic

activity, especially that associated with certain enzymes called *ases* embedded in the membranes of cells, results in the extrusion of ions like sodium and calcium and an enhanced concentration of potassium within the cell. The difference between the chemical potential of sodium and potassium ions favours the development of a negative potential within a cell, and this is enhanced by a more permanent or 'fixed' distribution of negative charge associated with protein within the cell.

For the present purpose it is unnecessary to study the biochemical mechanisms that we have just mentioned in detail, but it is sufficient to note that that they result in an electrical potential within a living cell that is of the order of 100 mV below that of the extracellular fluid. The channels which permeate the membrane are so narrow that they can normally support a difference of potential of this magnitude between their ends, but nevertheless *the channels of the membrane are in an electrically metastable state*, and very sensitive to various events tending to restore stability. In Sect. 8.1 we have identified this as one of the crucial conditions to be satisfied if quantal phenomena are to become manifest at the macroscopic level! The other condition, that the electrolytic fluids within or outside the cell should be of macroscopic dimensions, is trivially satisfied. We conclude that the membrane of a cell is at least potentially an effective detector of submicroscopic phenomena.

8.2.1 The Cortex as a Quantal Turing Machine

Some insight into the mechanism of information processing by the cortex is obtained by regarding it as Turing machine. Turing made several very influential contributions to the theory of computing. One which is worth considering briefly was intended to expose detectable differences, if any, between the processing of information by an advanced computer and by a human being. In his well known paper, Turing described an 'imitation game' in which a human participant was invited to discriminate between the answers given to a series of identical questions put to a suitably programmed computer and to another human; of course, the answers given by the computer were not required to be truthful. In retrospect, the conclusion to be drawn from such an experiment is that it is not difficult to simulate both the intelligence and goal fixation displayed by humans, but that no classical computer could be expected to create new information. New information is, by definition, unprogrammable, but once created, can be added to a computer program, and the problem posed by Turing's 'game' therefore requires a more careful formulation. Turing did not envisage the development of a quantal Turing machine, which, according to present theory, would be necessary and sufficient for the true emulation of consciousness.

In another paper, Turing had the intention to clarify the limitations on what could be computed by macroscopic computing machinery, but incidentally provided a specification of computing machinery that is applicable to all

classical computers. The classical Turing machine is a control unit that performs processing (simultaneous scanning and writing) operations on a 'tape' consisting of a sequence of two-valued bits. It may be supposed that in each operation only one bit is scanned and possibly modified, and that the next operation is on an adjacent bit. The machine itself is a 'black box' that does not need to be described in detail, except to the extent that has an internal state that may also be modified at each stage of the processing. From these specifications it will seen that the tape contains at different times the input to and the output from the computer, while the machine incorporates the program.

The specifications of the corresponding quantal Turing machine are similar, except in two respects. The quantal generalization may be a parallel as well as a sequential processor, so that arbitrarily many different bits of the 'tape' may be processed simultaneously. However, the more important difference is that the tape of the quantal machine consists of qubits instead of ordinary two-valued bits and the machine itself must therefore implement the logic of quantum mechanics rather than classical logic.

The usual approach to the more detailed specification of such machines has been to identify a quantal observable, such as the spin angular momentum of a microscopic system, as the content of the tape of the quantal Turing machine. The 'tape' would then be a microscopic system, and the machine would need the ability to detect and change the state of this microscopic system. If the chosen observable were selected the tape would be similar to the tape of a classical machine, except for the possibility of parallel processing. But more generally the tape would consist of qubits in an indeterminate state, and then that the results of the operation of the machine, though strongly correlated, would be *in principle* unpredictable and uncomputable. With the application to the animal cortex in mind, we shall next show that a thin, but not necessarily submicroscopic, layer of electrolyte can function as the tape of a quantal Turing machine, and shall subsequently give a quantitative account of a particular mechanism by which such a 'tape' may be read or modified by the machine.

8.2.2 The Qubits of Potential Fluctuations in an Electrolyte

In a resting state of an electrolyte there are no internal macroscopic currents and the macroscopic electric field is static, but at the microscopic level there are always fluctuations in potential and in states other than a resting state the fluctuations reach macroscopic proportions, especially in the surface layers of the electrolyte. The fluctuations of the potential φ are associated with fluctuations in the charge density ϵ arising from the motion of the ions, and can be calculated using Poisson's equation $\nabla^2\varphi = -\epsilon$, which though derived from Coulomb's law of electrostatics has a perfectly general validity in the Coulomb gauge adopted in most non-relativistic applications of classical and quantum electrodynamics. There is no need to use a relativistic theory in

this context, but we shall make use of quantized field theory by adopting expressions like (6.12) for the set of field variables ψ_a (a =H^+, OH^-, K^+, Na^+, Ca^{++}, Cl^-, ...) used to construct the charge densities ϵ_a and other observables for the various types of ions in the electrolyte. We shall show in this way that the potential φ is an observable with components $\tilde{n}_{b,l}$ that are, or consist of qubits and can be considered to form the tape of a quantal Turing machine.

The quantized charge density of ions of the b-the type is $e_b\psi_b^\dagger\psi_b$, and Poisson's equation can therefore be formulated as

$$\nabla^2\varphi = -4\pi\epsilon = -4\pi\sum_b e_b\psi_b^\dagger\psi_b, \tag{8.24}$$

with the electric charge density ϵ at the point $\mathbf{x}$ and time t expressed in terms of ionic components.

The field variables, written $\psi_b(\mathbf{x})$ and $\psi_b^*(\mathbf{x})$ when regarded as functions of position, are matrices, but, as in (6.17), can be in terms of sets of orthonormal functions $\chi_l(\mathbf{x})$ and $\chi_l^*(\mathbf{x})$ of position within the electrolyte:

$$\psi_b(\mathbf{x}) = \sum_l c_{b,l}\chi_l(\mathbf{x}) \qquad \psi_b^\dagger(\mathbf{x}) = \sum_l c_{b,l}^\dagger\chi_l^*(\mathbf{x}). \tag{8.25}$$

The individual terms in this expansion are eigenfunctions of the momentum and energy, and the quantized amplitudes $c_{b,l}$ are therefore periodic functions of the time. In fact later in this section we shall confirm that, in the context of the corresponding macroscopic theory, the potentials can be expressed as a sum of periodic functions of time. In the quantized theory, the $c_{b,l}$ are matrices which, depending on whether the a-the type of ion is a fermion or a boson, satisfy the (anti-)commutation relations

$$c_{b,l}c_{b,m}^\dagger \pm c_{b,m}^\dagger c_{b,l} = \delta_{l,m}, \tag{8.26}$$

of (6.27) and (6.39), from which it follows that any eigenvalue of the matrix

$$\tilde{n}_{b,l} = c_{b,l}^\dagger c_{b,l} \tag{8.27}$$

must be a non-negative integer. If the ions of the b-th type are fermions, the eigenvalue of $\tilde{n}_{b,l}$ can only be 0 or 1; if they are bosons, any non-negative integer is theoretically possible. In fact some of the ions in a typical electrolyte are fermions and others are bosons, but even for the bosons, at ordinary temperatures most of the eigenvalues of the $\tilde{n}_{b,l}$ are zero and the probability of finding an eigenvalue greater than 1 is negligible, so that the observables $n_{b,l}$ may be assumed to satisfy the characteristic equation

$$\tilde{n}_{b,l}^2 = \tilde{n}_{b,l}. \tag{8.28}$$

Like the $c_{b,l}$, the matrix elements of $\tilde{n}_{b,l}$ vary periodically with the time, in general. In other applications where eigenvalues of the boson numbers may

be greater than 1, it is of course still possible to express the observables in terms of qubits by the method of Sect. 4.4.

Although the above equation is sufficient to identify the $\tilde{n}_{b,l}$ as qubits, they determine the ionic densities and are not, therefore the qubits $n_{b,l}$ of the potential φ which we shall ultimately regard as forming the 'tape' of the quantal Turing machine. We shall therefore apply a unitary transformation to express the potential in terms of the $n_{b,l}$. According to (8.24), the microscopic charge density at he point $\mathbf{x}$ is given by

$$\epsilon(\mathbf{x}) = \sum_{b,l,m} e_b c_{b,l}^\dagger c_{b,m}\chi_l^*(\mathbf{x})\chi_m(\mathbf{x}), \tag{8.29}$$

and if f_{lm} is the solution of the equation

$$\nabla^2 f_{lm} = 4\pi\chi_l^*\chi_m \tag{8.30}$$

which tends to zero outside the electrolyte, the electrostatic potential at the same point is therefore

$$\varphi(\mathbf{x}) = \sum_{b,l,m} e_b c_{b,l}^\dagger c_{b,m} f_{lm}(\mathbf{x}). \tag{8.31}$$

We now introduce a matrix f (usually infinite) whose element in the l-th row and m-th column is f_{lm}. It follows from (8.31) that f is hermitean ($f_{lm}^* = f_{ml}$), and it can therefore be reduced to diagonal form by applying a unitary transformation, thus: $f \to ufu^\dagger$, where $(ufu^\dagger)_{lm} = f_m\delta_{lm}$ and $u^\dagger u = 1$. The elements $u_{lm}^\dagger = u_{ml}^*$ of the matrix $u^\dagger$ are obtained explicitly, together with the f_m, as eigenvectors and eigenvalues respectively of the matrix f:

$$\sum_k f_{lk}u_{km}^\dagger = f_m u_{lm}^\dagger \qquad \sum_k u_{lk}^\dagger u_{km} = \delta_{lm}. \tag{8.32}$$

Of course both the unitary matrix $u^\dagger$ and the eigenvalues f_l are functions of position and time in general. As $f_{lm} = \sum_k u_{lk}^\dagger f_k u_{km}$, the expression (8.31) for the potential reduces to

$$\varphi(\mathbf{x}) = \sum_{b,k} e_b n_{b,k} f_k,$$

$$n_{b,k} = \bar{d}_{b,k}d_{b,k}, \qquad \bar{d}_{b,k} = \sum_l c_{b,l}^\dagger u_{lk}^\dagger \qquad d_{b,k} = \sum_l c_{b,l}u_{kl}, \tag{8.33}$$

where, because of the unitary condition of (8.32), the $d_{b,k}$ and $\bar{d}_{b,k}$ satisfy the same relations

$$d_{b,l}\bar{d}_{b,m} \pm \bar{d}_{b,m}d_{b,l} = \delta_{l,m},$$

as the $c_{b,m}$ and $c_{b,m}^\dagger$ in (8.26). It follows that

$$n_{b,k}^2 = n_{b,k} \tag{8.34}$$

and we may identify the $n_{b,k}$ as qubits of a tape, in terms of which the potential can be represented simply and directly as shown in (8.33). In general, $n_{b,k}$ depends on the position $\mathbf{x}$ and the time t.

Our conclusion, then, is that *the quantized amplitudes $n_{b,k}$ of components of the potential in the electrolytic fluid of the cortex are qubits, and may be regarded as qubits of a 'tape' in a quantal Turing machine.* The measured value of any bit $n_{b,k}$, as might be found by scanning the tape, must of course be one of the binary digits 0 and 1. There is, in principle, no limit to the number of bits that can be scanned in the same measurement, and since the number (l) of different orthonormal functions, introduced in (8.25), is unlimited, the information to be gained from such a measurement is also unlimited.

There is no reason why it should not be possible to construct a variety of artificial devices with the essential properties of a quantal Turing machine with an electrolytic fluid as the 'tape' and an electrically metastable system as the 'black box'. To emulate consciousness, however, it would be necessary to provide the machine with a memory of information gained and the capacity to create new information on the 'tape'. These are the essential functions of the system of cells forming the cortex, and if we are to implement our characterization of the cortex as a quantal Turing machine, it still remains to be explained how the cells can be regarded collectively as the control unit of the machine. This will be done next, by studying the interactions between a cell and the electrolyte that are responsible for processing the 'tape'.

8.2.3 Transmission of Information Across the Cellular Membrane

Our next object will be to analyse qualitatively and quantitatively, the process of amplification of fluctuating microscopic potentials in transmission across the cellular membrane. Since this results in the development of potentials of several mV at the opposite surface of the membrane, the macroscopic formulation of the theory of electrolytes presented in Sect. 5.8 will be used, but since this is completely compatible with a microscopic formulation there will be no real limitation in doing so. The mechanism of amplification involves the influx or efflux of ions through the electrolytic channels that are a common feature of the unmyelinated cell membrane which forms the 'grey matter' of the cortex. Even the myelinated fibres that transmit action potentials between distant cells have nodes at intervals along their length that allow the passage of ions. The channels are not more than a few Ångstroms in diameter, and they cannot be detected by ordinary microscopy. However, their existence has been amply confirmed by observing the passage of radioactive tracer ions the across the membrane, and even more directly by the detection of currents by microelectrodes introduced near specific locations in the membrane. The independence of the currents carrying ions of different

types has led to the characterization of channels as calcium channels, sodium channels, chloride channels and potassium channels, and there is independent evidence that channels favour, even if they are not dedicated to, the transport of ions of a particular type.

Channels through the membrane are known to play an important part in synaptic transmission, so that submicroscopic effects could well modulate the process of the transmission of electrically and chemically coded information at synapses between cells in the nervous system, which has usually been described in the literature in macroscopic terms. Synaptic transmission is known to require an influx of calcium ions into the postsynaptic cell, released from the external surface of its membrane by the interaction of neurotransmitter molecules with enzymes embedded in the surface. This is certainly a macroscopic process, but the fact that much synaptic transmission is synchronized with potentials in the extracellular environment suggests that even where purely macroscopic synaptic processes are involved, quantum mechanical effects play a role in the nervous living animal.

What is known about the geometry of the internal surface of the channels suggests that they are approximately cylindrical in shape but that the entrances to the channels are somewhat indented in the membrane so that their length is of the order of 50 Å and somewhat less than the normal thickness of the membrane. The dimensions of the channels are such that they cannot accommodate more than a small number of ions at a time, and it is therefore quite appropriate to represent the transmission of the ions, and propagation of the electrical and ionic potentials through the membrane, as a quantum mechanical process. The channels are the interface between a cell and the extracellular fluid and are widely distributed over the surface of the membrane, so that the associated processing of information is largely parallel, though sequential processing is certainly involved in any subsequent development of rather large ionic currents associated with graded and action potentials within the cell, as in the generation of much smaller external currents which contribute to fluctuations in the extracellular field.

The theory of Debye–Hückel given in Sect. 5.8 will now be generalized for electrolytes that are not necessarily in thermodynamical equilibrium. To obtain explicit time dependent solutions of we shall need to take into account the variation with time of the charge density. This can always be expressed in terms of the chemical potentials, and while in thermodynamical equilibrium the latter depend only on the position $\mathbf{x}$, more generally they vary with time.

In the quantitative theory of the transmission of potentials through channels in the cellular membrane, the important physical variables are the electric potential φ, the ionic charge densities ϵ_a and the corresponding current densities $\mathbf{j}_a$, and here these will be understood to be expectation values computed with the statistical matrix. The averaging implied by the taking of expectation values does not affect the validity of any of the linear relations between the physical variables fields such as Coulomb's law, the laws of conservation

of the various types of ions, and the generalization of Ohm's law which determines the currents. For convenience we now collect together the equations which are the mathematical expression of these laws, corresponding to (5.85), (5.86), (5.81) and (5.83) respectively:

$$\nabla^2\varphi = -(4\pi/\kappa)\sum_a \epsilon_a, \qquad \epsilon_a = \epsilon_a^0 \exp(-\beta e_a \varphi_\alpha), \qquad \epsilon_a^0 = e_a n_a^0,$$

$$\frac{\partial \epsilon_a}{\partial t} + \nabla \cdot \mathbf{j}_a = 0, \qquad \mathbf{j}_a = -\sigma_a \nabla(\varphi - \varphi_a). \tag{8.35}$$

In the last equation σ_a is the electrical conductivity, proportional to ϵ_a, and $\varphi - \varphi_a$ is the electrochemical potential of ions of the a-the type. The ϵ_a^0 are charge densities of the resting state, and may vary rather rapidly with position in the channels of the membrane, but not in the extracellular or intracellular electrolytic fluids. By the summation of the last equation with respect to a, we obtain we obtain the generalized Ohm's law

$$\mathbf{j} = \sum_a (\sigma_a \nabla \varphi_a) - \sigma \nabla \varphi, \qquad \sigma = \sum_a \sigma_a,$$

where σ is the overall conductivity of the electrolyte.

By differentiating the expression for ϵ_a in (8.35) with respect to time and the elimination of the charge and current densities from these equations, we now obtain a set of relations, not restricted to thermodynamical equilibrium, between the electrical and chemical potentials. In the elimination of $\mathbf{j}_a$, the term $\nabla\sigma_a \cdot \nabla(\varphi - \varphi_a)$ may be consistently neglected since terms involving products of gradients are already assumed to be negligible in the derivation of Ohm's law. Since the ionic conductivities σ_a are proportional to the corresponding charge densities ϵ_a, assuming that the latter are not too large, we may introduce *resistance constants* γ_a by writing

$$\sigma_a = \beta e_a \epsilon_a / \gamma_a; \tag{8.36}$$

then, neglecting the term , we obtain

$$\frac{\partial \epsilon_a}{\partial t} = \beta \epsilon_a \nabla^2(\varphi - \varphi_a)/\gamma_a = -\beta e_a \epsilon_a \frac{\partial \varphi_a}{\partial t},$$

or

$$\gamma_a \frac{\partial \varphi_a}{\partial t} = \nabla^2(\varphi_a - \varphi). \tag{8.37}$$

Also, the elimination of ϵ_a from (8.35) gives

$$\nabla^2\varphi = (4\pi/\kappa)\sum_a \epsilon_a^0 \exp(-\beta e_a \varphi_a). \tag{8.38}$$

With suitable boundary conditions, the last two equations are sufficient to determine all the potentials in an electrolyte.

The equations obtained for the potentials are non-linear, but the non-linearity is important only in the calculation of action potentials where deviations from the resting state exceed 10 mV, and an approximation which reduces (8.38) to a form linear in the potentials is quite sufficient for our present purpose. The charge densities ϵ_a^0 of the resting state satisfy the condition $\sum_a \epsilon_a^0 = 0$ for electrical neutrality, so that when the exponential function in (8.38) is replaced by $1 - \beta e_a \varphi_a$ the resulting equations are then

$$\gamma_a \frac{\partial \varphi_a}{\partial t} - \nabla^2 \varphi_a = -\nabla^2 \varphi = \sum_b C_b \varphi_b, \qquad C_b = 4\pi\beta e_a \epsilon_a^0/\kappa, \tag{8.39}$$

where C_b, like ϵ_b^0, varies only within the channels through the membrane. The electrostatic potential φ may clearly be determined from the same equations as φ_α by substituting $a = 0$, with $\varphi_0 = \varphi$ and $\gamma_0 = 0$.

For the solution of (8.39) we shall need estimates of the way the ionic concentrations C_b in the resting state, i.e., the state of metastable equilibrium, vary from within the extracellular fluid and through the channels in the membrane as far as the interior of the cell. According to (8.35), these concentrations are related to corresponding values φ_a^0 of the chemical potentials, and since, in the resting state, the ionic currents are zero, the chemical potentials differ only by constants from the electric potential φ^0. The latter satisfies the Debye–Hückel equation of (5.90), so that

$$\nabla^2\varphi^0 = \frac{\partial^2 \varphi^0}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \varphi^0}{\partial r}\right) = a_{\mathrm{D}}^{-2}\varphi^0 \tag{8.40}$$

in cylindrical coordinates, where z is a distance normal to the membrane surface, conveniently measured from a point midway across the membrane, and r is a radial coordinate, measured where appropriate from the axis of a channel. The differential equation has solutions of the form

$$\varphi^0 = \varphi_{\mathrm{e}}^0 + \varphi_{\mathrm{f}}^0 \exp(\pm z/a_{\mathrm{D}}),$$

$$\varphi^0 = \varphi_{\mathrm{g}}^0 z/(2d) + \varphi_{\mathrm{h}}^0 K_0(\alpha r)\sin(\pi z/d),$$

where $K_0(\alpha r)$ is a modified Bessel function of the second kind. The first can be used near a surface of the membrane, if the constant φ_{e} is chosen to be the potential within the electrolyte at some distance from the surface. The second solution could be useful within channels of the membrane and may be used to obtain corresponding expressions for the C_b in (8.39), but these are rather complicated and hardly necessary to represent the variations over such a small distance. In the following we shall therefore approximate the concentrations within a channel of the membrane by

$$C_b(z) = C_b^m + C_b^d \sin(\lambda z), \tag{8.41}$$

where $\lambda = \pi/d$ and $2d$ is the length of the channel. The value of λ is chosen to match the almost constant values $C_b^m \pm C_b^d$ for $z = \pm\frac{1}{2}d$ outside the

membrane, so that C_b^m is a mean value and $2C_b^d$ a difference of values in the internal and external electrolytic fluids.

We shall look for periodic solutions of angular frequency ω of the equations (8.39), and again adopt cylindrical coordinates z and r within a channel, where z and r measure longitudinal and radial distances from the midpoint of the axis of the channel. The coordinate z takes values between $-\frac{1}{2}d$ and $\frac{1}{2}d$, where d (~ 80 Å) is the thickness of the membrane. With these coordinates, we write

$$\varphi_a = \Re\left[e^{i\omega t} J_0(\alpha r)\psi_a(z)\right], \tag{8.42}$$

where $\Re$ denotes the real part of the expression that follows, and $J_0(\alpha r)$ is the Bessel function of order 0, satisfying

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial J_0(\alpha r)}{\partial r}\right) = -\alpha^2 J_0(\alpha r).$$

If $\alpha/r_c = 2.406$, the value of the first zero of the Bessel function, then φ and φ_a will vanish for $r = r_c$, on the internal surface of the channel. On substituting (8.42) into (8.41), and using the expression for the Laplacian ∇^2 given in (8.40)we have

$$-\frac{d^2\psi_a}{dz^2} - (\alpha^2 + i\omega\gamma_a)\psi_a = \chi, \qquad \chi = \sum_b C_b(z)\psi_b. \tag{8.43}$$

With C_b given by (8.41), (8.43) is a generalization of Mathieu's equation and can be solved by writing

$$\chi = \sum_{j=-\infty}^{\infty} \chi_j \exp(\mu_j z), \qquad \mu_j = ij\lambda + \epsilon;$$

$$\psi_a = \sum_{j=-\infty}^{\infty} \psi_{aj} \exp(\mu_j z), \tag{8.44}$$

where ϵ may be regarded as a dynamical analog of the inverse Debye shielding distance in the electrolytic channels. When (8.44) is substituted into (8.43), the latter is satisfied, provided that the coefficients ψ_{aj} are given by

$$\psi_{aj} = \frac{\chi_j}{\mu_j^2 - \alpha^2 - i\omega\gamma_a},$$

$$(1 - f_j)\chi_j = g_{j-1}\chi_{j-1} - g_{j+1}\chi_{j+1}, \tag{8.45}$$

with

$$f_j = \sum_b \frac{C_b^m}{\mu_j^2 - \alpha^2 - i\omega\gamma_b}, \qquad g_j = \frac{1}{2i}\sum_b \frac{C_b^d}{\mu_j^2 - \alpha^2 - i\omega\gamma_b}. \tag{8.46}$$

A theory of fluctuations of potentials near the surface of the membrane in the extracellular and intracellular fluids, to be given in the next section, can be recovered from these results. Complex values of λ_j are determined as functions of the real angular frequency ω, from a dispersion equation of the form $f_j = 1$, and the detailed analysis shows that a continuous spectrum of angular frequencies within certain bands is available. The solutions may be classified as resonances associated with particular ions, present in low concentrations, such as calcium and sodium within the cell, or calcium and potassium outside the cell.

However, because of the need to match boundary conditions in the extracellular and intracellular fluids, there are quite severe constraints on the solutions in the channels of the membrane. In general the solutions (8.44) of (8.43) are unacceptable, because the infinite series in the former are badly divergent. However there are convergent solutions for special values of ω and ϵ, determined from the condition that χ_j should decrease like j^{-2} for large values of j. These solutions may be computed by a method which neglects χ_j for $j > J$, where $J \geq 5$, chooses any small but non-zero value of χ_J and solves the difference equation of (8.45) with a succession of pairs of eigenvalues (ω, ϵ), until a negligible absolute value of χ_{-J} is obtained. It can be verified that the eigenvalues are insensitive to the choice of J. In this way it is not difficult to compute pairs of eigenvalues (ω, ϵ), and the corresponding potentials. The values of the concentrations C_b^m and C_b^d are taken from observation and the values used for the resistance constants γ_a are the same as used to model graded and action potentials in the cytoplasm. The assumed geometry of the channels is consistent with recent experimental investigations.

For values of the radius r_c of the channel of the order of 5 Å, there is a static solution with $\omega = 0$ and $\psi_a = \psi$, but ψ varies with distance across the membrane. The existence of this solution is in agreement with the observation of metastable potentiated states of the cell membrane with a range of potential differences between its internal and external surfaces. The more general solutions with $\omega \neq 0$ show an amplification, by a factor of the order of 10^6, of potentials along a channel, so that microscopic fluctuations of the order of 1 nV at one end are amplified to fluctuations of the order of 1 mV at the other end. The lower frequencies all lie in bands associated with various rhythms, known as the θ-rhythm, the α-rhythm and the β-rhythm, observed in EEG recordings.

If ω is an eigenvalue, so is $-\omega$, and if ϵ is an eigenvalue, so is $-\epsilon$. Reversing the sign of ϵ reverses the direction of amplification, and to satisfy boundary conditions at both surfaces of the membrane a combination of two solutions with equal and opposite values of ϵ is normally required. Thus, if information can be gained by the cell at a particular frequency, it can also be created, and *it is normal for information to be gained and created by the same process.* But for the sake of clarity Fig. 8.1 shows a gain of information by the cell, with a potential gradient approaching zero at the outer membrane surface.

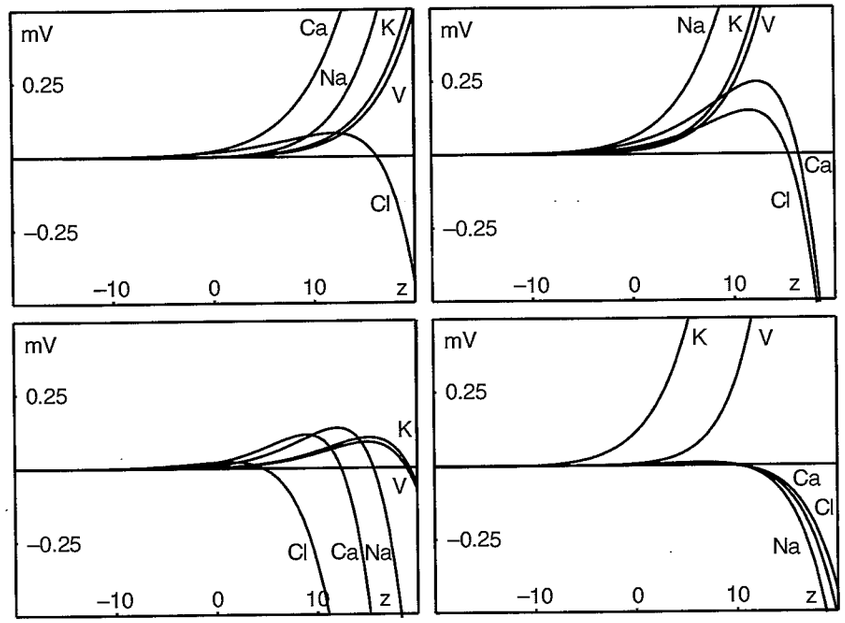

Fig. 8.1. Amplitudes of a small potential $V = \Re\psi$ and the corresponding chemical potentials (K, Na, Ca and Cl) for time $t = 0$, as functions of distance through calcium, sodium, chloride and potassium channels (top left to bottom right, respectively) of the neural membrane, corresponding to some of the lowest eigenvalues of the frequency.

Figure 8.1 shows the variation with distance across the membrane of all potentials for four different non-vanishing eigenvalues of the angular frequency, the first, second, third and sixth in ascending values of ω. The different curves serve to illustrate the amplification of all potentials in transmission through a channel in the membrane. The coordinate z takes values from -20 to 20 Å in the internal region shown. The first set of curves, at top left, is clearly for a calcium channel and corresponds to the eigenvalue $\omega \simeq 31\ \mathrm{s}^{-1}$(or 5 Hz, matching the θ-rhythm) of the angular frequency. Oscillations and waves of calcium are in fact observed within a wide variety of cells, as well as in the extracellular fluid. An influx of calcium similar to that shown marks the initial stage of the development of a graded or an action potential. From (8.35) it is evident that the calcium current is proportional to the gradient of the calcium and electric potentials, and this is therefore inwardly directed. Calcium is known to be transmitted by many different electrolytic channels, and is essential for the subsequent exchange of sodium and potassium across the membrane. Beyond the point where the amplitude of fluctuations of any of the potentials exceeds a value of 20 mV, the oscillations become non-linear and are not necessarily periodic.

There are other modes, corresponding to larger frequencies, which show an even larger amplification of the potentials across the membrane, and are also dominated by ions of a particular type. The mode corresponding to the second non-zero eigenvalue, $\omega \simeq 45\ \mathrm{s}^{-1}$ (7 Hz, near the upper limit of the θ-band) is also shown at top right in Fig. 8.1. This mode is obviously dominated by sodium ions, and corresponds to a sodium channel, though there are other eigenvalues corresponding to frequencies of 16 Hz, in the α-band, and 29 Hz in the β-band. Of course these frequencies depend rather sensitively not only on the assumed concentrations, but also on the geometry of the channel, so that some variability of the frequencies associated with different channels should certainly be expected. Sodium channels play an important role in the initial stages of the influx of sodium which follows the influx of calcium in the development of an action potential, though in that process non-linear effects become very important.

The sets of curves at bottom left and bottom right in the figure correspond to other low-lying eigenvalues of the angular frequency, respectively to a chloride channel at 10 Hz in the α-band and another sodium channel, and a potassium channel at 57 Hz. There are also eigenvalues at still higher frequencies, and positive indications that some of the higher frequencies play a significant part in the formation of memory.

We have thus been able to model some of the early macroscopic consequences of the detection of a bit, which were earlier described in quantal terms. The results have important implications for the activation of neurons by potentials in the extracellular fluid, but also imply the creation of new information in the extracellular fluid through the amplification of microscopic potentials originating within the cells of the cortex. It remains to examine some of the macroscopic consequences of this transfer of information.

8.3 Cells and Membranes

We next summarize some of the more relevant facts concerning individual cells of the enormous system of symbiotic cells that constitute the animal cortex, derived from a wide variety of experimental investigations. In doing so we should recognize that any cell has metabolic and reproductive functions which are essential to life, but at present we more concerned with the electrochemical processes that allow them to communicate with one another.

We have already seen that the cells which make up the nervous system of an animal, and the brain in particular, are surrounded by a layer of electrolyte, about 150 Å thick and consisting mainly of an aqueous solution of sodium, potassium and chloride, somewhat similar in composition to the sea water in which life is believed to have originated. The extracellular fluid has also a very small and variable but important concentration of free calcium, as well as calcium that is loosely bound to receptor molecules at the surface of the membranes by which each cell is bounded. The membrane of a cell

is composed mainly of bilipid material about 80 Å thick, but is permeated by channels which, though only several Å in diameter, allow the passage of ions under certain conditions. The *cytoplasm*, or internal fluid of the cell, is also an electrolyte, considerably richer in potassium than the extracellular fluid but depleted in sodium as the result of the ongoing exchange of internal sodium for extracellular potassium which is mediated by enzymes in the membrane and supported by the metabolism of the cell. As a result of this activity, the electrostatic potential in the cytoplasm is normally 50–100 mV below the potential in the extracellular fluid.

The transfer of information from one cell to another is necessarily through the extracellular fluid. An important component of this transfer occurs at *synapses* which form part of the extracellular fluid but have a specialized capacity to activate the postsynaptic cell. This activation is most obviously the result of a transient influx of sodium and efflux of potassium through specialized channels in the synaptic membrane of the cell, but is initiated by calcium released from the membrane surface by the action of neurotransmitter substances which originate in the presynaptic cell.

Some of the synapses which transmit information leading to the activation of a cell may be localized on the *soma* or cell body, but in many cells are at the external surfaces of a system of *dendrites* which, like the tributaries of a river, convey potentials from a variety of synaptic sources to the soma. Information is normally transmitted by a cell to many other cells by an action potential which propagates from the soma along the *axon* of the cell, which ultimately branches so as to reach a multiplicity of presynaptic surfaces. In the nervous system of insects cortical function is more rudimentary and there is a greater reliance on local feedback mechanisms, so that the distinction between dendrites and axons is often blurred. But in animals it is remarkable that within the axonic and dendritic processes of cells of the nervous system, information is always channeled to and from synapses in a certain direction, from dendrites to axon and by afferent fibres of the presynaptic cell to the postsynaptic cell.

Within a postsynaptic cell activation results in fluctuations of electrostatic potential, sooner or later affecting the soma and the axon of the cell. The activation begins as a *graded potential* of a few mV, but develops under suitable conditions into an *action potential* of the same order (50–100 mV) and opposite in sign to the internal potential of the cell. Thus both graded action potentials tend to restore the potential difference between the cell and its environment. For a graded potential to develop into an action potential it must reach or surpass a certain threshold value.

Fluctuations of potential within a cell may be quite large especially in action potentials, and are accompanied by fluctuations of a few mV in the extracellular fluid. But there are also extracellular fluctuations not obviously related to intracellular activity. These fluctuations may be detected by metallic probes, but less intrusively by pasting electrodes on the surface of the scalp.

The electroencephalogram (EEG) was invented by Berger to monitor fluctuations of potential at or near the surface of the cortex, and the very small electric currents which accompany them may also be detected by magnetoencephalogram (MEG) and nuclear magnetic resonance (NMR) techniques. Although a close correspondence was soon apparent between EEG and MEG records and certain patterns of mental activity, at a time when there was no deep understanding of the workings of the brain, it was assumed that the potentials recorded represented a mere by-product of the processing of information by the cells of the cortex rather than an essential contribution to the transfer of information. But later experimental investigations in which EEG recordings were obtained from a number of locations distributed over the surface of the human scalp showed a direct relation between patterns of extracellular potentials and conscious activity; even where fluctuations in extracellular potential were apparently random, careful analysis revealed the underlying presence of characteristic frequencies associated with particular types of conscious activity. Moreover, a variety of evidence steadily accumulated leading to the conclusion that the extracellular potential was capable of influencing, as well as being influenced by, the internal activity of the cells, so that synaptic transmission was not the only means of communication between cells.

The volume of experimental evidence that individual cells and groups of cells of the animal cortex are selectively sensitive to particular frequencies gives no reason to doubt that small fluctuating components of the extracellular field are at least contributory to conscious activity, the effects of which can be observed. It might be thought that if potentials transmitted through the extracellular fluid could influence the activity of cells, their effect would be widespread and unacceptably chaotic. But in the previous section it has been shown there must be a synchronization of cellular activity with extracellular potentials with a particular frequency; the effect of such potentials is not at all indiscriminate and in fact favours an orderly sequence of events at the macroscopic level. Moreover, in view of our demonstration in Sect. 8.2 that such components can be represented as qubits, a mechanism is readily apparent for the escalation of indeterministic quantum mechanical events to the macroscopic level of graded and action potentials. In fact nearly all existing theories of consciousness accept that much of the macroscopic activity of the brain is indeterministic and unpredictable. Although action potentials, which are the effective means of transmission of information over considerable distances within cells, are macrosopic phenomena, they develop from very much smaller potentials. Thus, notwithstsanding the fact that submicroscopic events which influence the development of macroscopic potentials inevitably escape notice; their macroscopic consequences are accessible to experimental observation. We shall now proceed to a quantitative theory of the potentials at the cellular level.

8.3.1 Graded and Action Potentials

To model the rather large fluctuations of potential within a cell we make use of the equations (8.37) and (8.38) for the electric potential ($\varphi_0 = \varphi$) and ionic potentials (φ_a). These equations we first rewrite in the form

$$\gamma_a \frac{\partial \varphi_a}{\partial t} - \nabla^2 \varphi_a = \chi, \qquad \chi = (4\pi/\kappa) \sum_b \epsilon_b^0 \exp(-\beta e_b \varphi_b), \tag{8.47}$$

recalling that κ is the dielectric constant (~ 80 for aqueous electrolytes) and $\beta = 1/(kT)$ is inversely proportional to the absolute temperature (T). Except for $\gamma_0 = 0$, the coefficients γ_a may be interpreted as ionic resistances, and the ϵ_b^0 are the corresponding charges densities. We are interested in solutions in electrolytic fluid near the internal surface of a cellular membrane, where the ϵ_b^0 can be treated as constants.

The equations (8.47) are non-linear but, they can be solved to any desired degree of accuracy by suitable numerical methods. So long as the ionic potentials φ_a do not exceed ~ 10 mV, the linearization of the expression χ used in (8.39) is permissible:

$$\chi = \sum_b C_b \varphi_b, \qquad C_b = 4\pi\beta e_a \epsilon_a^0/\kappa, \tag{8.48}$$

where the C_b are now constants. We shall obtain particular solutions with an angular frequency ω of the linearized equations for φ_a obtained from (8.47) and (8.48), by expressing φ_a as the real part of a complex function $e^{i\omega t}\psi_a$ that is also an eigenfunction of the Laplacian ∇^2, thus:

$$\varphi_a = \Re(e^{i\omega t}\psi_a), \qquad \nabla^2 \psi_a = (q + i\omega p)\psi_a. \tag{8.49}$$

More general solutions may then be obtained as a linear combination of the particular solutions for different values of ω.

As can be seen from the substitution of the particular value 0 of ω, the constant q in (8.49) can be regarded as a generalization the inverse square Debye shielding distance a_D^{-2}, and p as a measure of the mean resistance of the electrolyte, for fluctuations of frequency ω. In fact we can verify that there are two relations connecting ω, p and q, as follows. If (8.48) is substituted into (8.47), we obtain the algebraic equations

$$[q + i\omega(p - \gamma_a)]\psi_a = \sum_b C_b \psi_b = \chi', \text{ say,} \tag{8.50}$$

to determine the ionic potentials. We can assume that ω is real, since otherwise the solution would become unacceptably large for large positive or large negative values of the time t. When

$$\psi_a = \chi'/[q + i\omega(p - \gamma_a)]$$

is substituted into (8,50), the latter reduces to the condition

$$\sum_b \frac{C_b}{q + i\omega(p - \gamma_b)} = 1$$

which may then be separated into the two real algebraic equations

$$\sum_b \frac{qC_b}{q^2 + \omega^2(p - \gamma_b)^2} = 1, \qquad \sum_b \frac{(p - \gamma_b)C_b}{q^2 + \omega^2(p - \gamma_b)^2} = 0. \tag{8.51}$$

The most convenient method of solution is to choose some value of p, to use the second equation of (8.51) to determine q/ω; and then the first equation to determine q, and thus the corresponding value of ω.

When C_b is sufficiently small, and the frequency ω is such that the effective resistance p has a value sufficiently near to one of the ionic resistances γ_b, then the value of q is small, so that the effective shielding length is correspondingly large, and the corresponding denominators in (8.51) are small, and, in the terminology of dispersion theory, the condition for a *resonance* is satisfied. We note here that such resonances are associated with ions like calcium which have small concentrations. Such resonances play an essential part in the development of graded and action potentials.

When the ionic potentials exceed values of a few mV, the accuracy obtained by linearization of the exponential factors in (8.47) becomes increasingly poor, so that the numerical integration of the non-linear equations is required. Some experimentation with initial values is needed to obtain stable solutions. A typical example of the curve obtained, representing an action potential, is shown in Fig. 8.2.

The integration of the non-linear equations for different calcium concentrations and other parameters and different initial conditions yields a variety of potential curves, some representing graded potentials of a few mV and some action potentials, of which Fig. 8.2 provides an example. All curves closely resemble those observed in nature, where graded potentials are observed if a critical value known as the threshold value of the potential is not reached, but action potentials normally result if a cell receives activation from a sufficient number of sensitized synapses as well as from the extracellular fluid. A cell which has experienced an action potential, in which the internal potential reaches a characteristic value, is said to have 'fired'. Several types of action potential are possible:

(1) After firing, the cell may enter what is known as a refractory state with a potential well below the resting potential, in which it is quite insensitive to further activation. If, as in Fig. 8.2, its recovery is sufficiently rapid, the refractory state is short-lived and after passing the resting state it is possible for the threshold to be exceeded, so that the action potential is followed by one or more further action potentials. If the resting potential but not the threshold potential is exceeded, the action potential is followed by a graded potential.

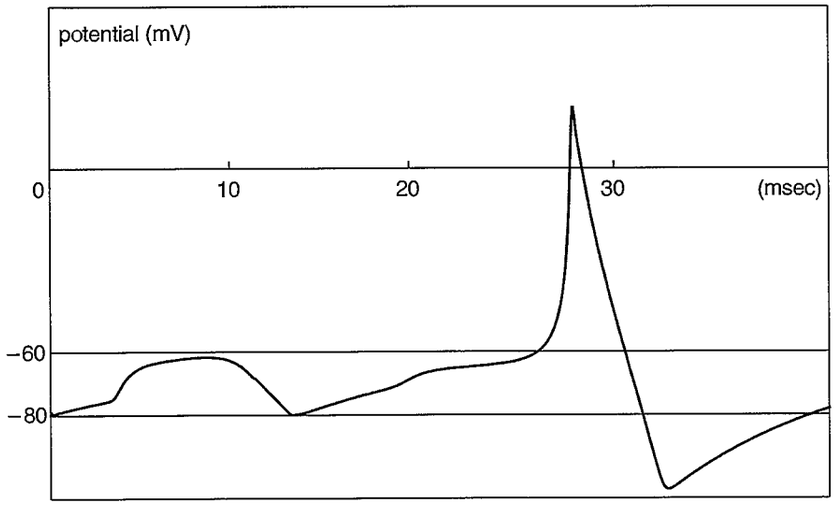

Fig. 8.2. Computed action potential, showing rapid rise in potential within the cell after passing the threshold value, and slow return to resting value in the refractory state which follows.

(2) The recovery in the refractory state may last for many microseconds, and the potential within the cell then approaches the resting potential without exceeding it.

(3) After firing, the cell may remain for an indefinite time in a potentiated state with a potential intermediate between the resting potential and the threshold. This state is similar to those of long-term potentiation (LTP) which have been the subject of extensive experimental investigations.

Long-term potentiation is not necessarily associated with an action potential, or even a graded potential, but can be induced most effectively under experimental conditions by a combination of a weak synaptic stimulus, and a long sequence of equally spaced stimuli, mimicking one of the natural rhythms, such as the theta rhythm and the alpha rhythm, that are known to produce LTP. The importance of LTP stems from its role in the formation of memory. It has been found that the synapses of a neuron undergo a process of progressive electrochemical and physical development during LTP, so that they are sensitized and the cell receives greater activation and fires more readily as a result of subsequent synaptic stimuli. In the following section we shall describe how *this may lead to the periodic repetition of entire sequences of the action potentials that follow sensory and other activity in the cortex*. Such repetition may be construed as the formation and reinforcement of memory.

8.4 The Animal Cortex

In spite of the enormous complexity of the system of many billions of symbiotic cells which make up the human cortex, and the elaborate network of afferent and efferent fibres which allow them to communicate, it is made up of well defined structures the functions of which are by now are sufficiently well understood to allow relatively simple models to be constructed.

8.4.1 Organization of Cells in Columns and Zones

Individual neurons of the cortex have either an excitatory or inhibitory effect on other neurons, depending on the type of neurotransmitter that they release at their synapses. In the cerebrum the pyramidal cells are excitatory, but in the cerebellum the otherwise analogous Purkinje cells are inhibitory. The simplest structures are formed by the clusters of neighbouring cells that include or directly influence the action of the pyramidal cells or Purkinje cells, that are responsible for either initiating or providing essential input to most of the activity of the nervous system. These clusters form *columns* extending from near the surface of the cortex through a succession of layers containing cells of similar types.

A typical pyramidal or Purkinje cell lies fairly near the surface, and receives its principal excitatory activations from a much more numerous set of granule cells in a deeper layer, which are in turn activated by cells in more remote columns or nuclei. Often, as for Purkinje cells, there is also direct excitatory activation from distant cells. Apart from the granule cells, and the important cell providing the output of the cluster, a column contains a variety of *interneurons* that with one or two exceptions are inhibitory. Prominent, though not unique among the interneurons in most parts of the cortex are the inhibitory basket cells. Though the organization of the columns might appear to be unnecessarily complex, it does provide for a fine balance of excitation and inhibition to important cells that might otherwise be too active.

Somewhat more extended units in the more detailed organization of the cortex are called *zones* or *segregates*, defined as areas containing output cells that have a very similar function. Even larger units that have been identified are the areas associated with particular sensory and motor functions. But in order to discuss these functions adequately we shall next give a brief description of the overall organization of the cortex.

8.4.2 The Subdivisions and Functions of the Cortex

The cortex consists of all the surface layers of the brain, within an area augmented by the incorporation of a variety of protuberances and crevices, as well as the cavity called the lateral ventricle on each side of the head. The principal components are the cerebrum and the cerebellum, but worthy of

notice is the distinction between the neocortex and allocortex. The latter is the most primitive part of the cortex, and forms part of the limbic system but contains the hippocampus, which is situated just within the lateral ventricle, as shown in Fig. 8.3.

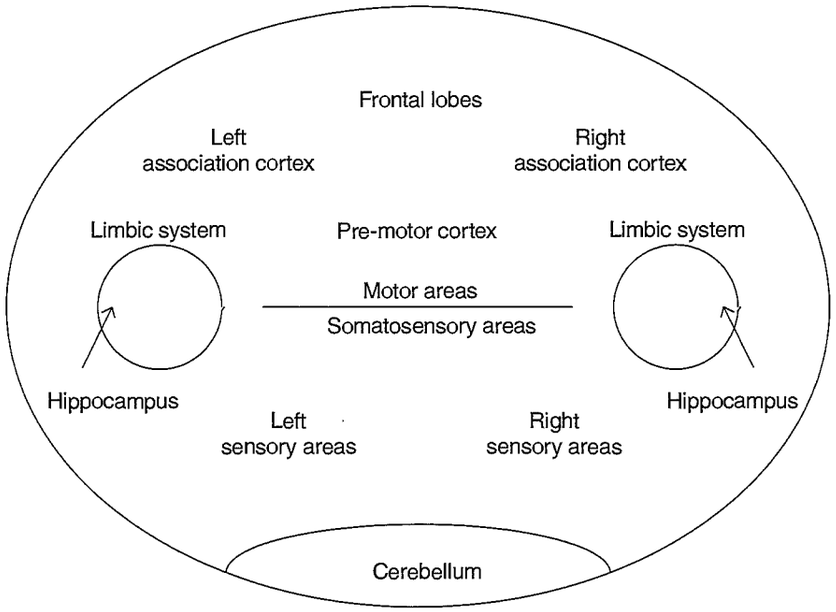

Fig. 8.3. Schematic representation of the surface of the cortex, showing the principal functional subdivisions.

In a relatively short period of evolution the neocortex of human beings has grown in size and structure to an extent that fully accounts for the superiority of mankind in a number of respects important for natural selection and survival. The principal difference between the cortices of humans and those of other primates and animals is in the development of association and frontal areas which are responsible for a number of functions. Prominent among the functions of the association areas is the power of recognition, the result of the formation of a very detailed sequential memory of visual sensory impressions, and also of the auditory impressions involved in interpersonal communication by speech. It is known that sensory stimuli are normally relayed from one hemisphere of the cortex to the other, and also that left and right areas have specialized functions related to recognition and comprehension. The frontal areas are the locus of a good deal of the mental activity that does not result in immediate motor action, and it is a reasonable inference, for which there is also considerable experimental evidence, that much conscious, as opposed

to unconscious, activity is in these areas. The left and right hemispheres are multiply connected by the *corpus callosum*, and severing the connections can result in the apparent creation of two separate centres of consciousness.

Motor activity is initiated in areas somewhat to the front and somatosensory and sensory areas somewhat to the rear of the midline. However, from early childhood motor activity is increasingly influenced by the inhibitory input of the cerebellum, from which the fine control of motor action gained as a result of learning and experience is derived. On the other hand, sensory information which needs to be remembered is channeled through the hippocampus. The limbic system is also largely responsible for the influence of the emotions on animal behaviour.

Our principal interest in the present context is in the creation of long-term memory, where it is known that the hippocampus plays an essential part though the actual memory resides elsewhere and may be rather widely distributed. The experience of people suffering temporary global amnesia, in which the functioning of the hippocampus is interrupted for several hours, shows that it is particularly important in the formation of *sequential* memory, as opposed to momentary impressions which would have little significance in isolation. Loss of memory extends for a day or two, though not longer, before a failure of hippocampal function, showing that the hippocampus is also important for the periodic and not necessarily conscious reinforcement of memory. To obtain some understanding of these and other observations, we discuss in terms of transfer of information a simple model of the mechanism by which the long-term memory of a sequence of sensory impressions is created. The information has its origin in a sequence of external events E_i $(i = 0, 1, 2, ...)$ such that E_{i+1} is closely related to E_i. The event E_i activates a set of sensory receptor cells R_i, which normally contains several neurons. The information represented by the firing of these cells is then transmitted to a corresponding set of sensory cells and thence to a set of already sensitized sensory association cells S_i. The firing of S_i potentiates and sensitizes not only the closely related set of cells S_{i+1} but activates a corresponding set of cells H_i of the hippocampus. The firing of the cells of the hippocampus is synchronized by the theta-rhythm in the extracellular fluid. The information represented by the firing of H_i is transmitted to and further sensitizes S_{i+1} which is then activated by R_{i+1}. Short-term memory of the sequence of events E_1, E_2, ... then requires only the activation of S_1 by S_0 and S_2, S_2 by S_1 and S_3, ... and similar repetitions of firings of closely related sensory association cells. If at some later time any cells of the sequence S_0, S_1, S_2 are consciously or unconsciously activated, and corresponding cells of the hippocampus are activated, the memory of the sequence of events will be reinforced, and as the result of reinforcement over a period of one or two days recall is possible by the activity of any of the now well sensitized sensory association cells without the participation of the hippocampus.

This and similar processes of memory formation can be simulated by computer programs designed for the sequential solution of a *neural network equation* of the type

$$a_j(t+\tau) = a_j(t) + r_j(t) + e_j(t)i_j(t) + \sum_k i_j(t)w_{jk}(t)o_k(t+\tau_k) \qquad (\text{mod } m). \tag{8.52}$$

For computational convenience, all quantities in this equation are integers, and the time t is a multiple of a fixed time interval τ, of the order of 1 microsecond. A subscript j is used to distinguish different neurons belonging to a network, and $a_j(t)$ is the *activation level* of the j-th neuron, representing the internal potential though not necessarily on a linear scale. In early neural network models, $a_j\,(t)$ had only two values 0 and 1, but the realistic representation of refractory states, the resting state and the firing states of a neuron requires as many as 9 values. The term $r_j(t)$ on the right set of neurons simulates the ascent from one level to the next in refractory states, where $i_j(t) = 0$, and $e_j(t)$ represents the extracellular input when $i_j(t) = 1$. The factor $w_{jk}(t)$ is the 'weight' of synapses from the k-th neuron to the j-th neuron and $o_j(t+\tau_k)$ has the value 1 or 0 according as there is or is not activation from the firing of the k-th neuron at time $t+\tau_k$, where $\tau_k = \tau$ or 0 according as $k < j$ or $k > j$. To represent the progressive sensitization of the synapses with use, the weights $w_{jk}(t)$ increase with a certain probability from a minimum value of 1 up to a prescribed maximum if $o_k(t+\tau_k) = 1$.

An important feature of the neural network equation (8.52) is the role of the extracellular potential in the sequence of events leading to motor activity, this has been described in some detail by Eccles, and can be simulated without much difficulty. The most important feature of such sequences is the continual access to inherited memory or memory developed earlier in the course of training. They could well have a role in the processes of *intelligence* and *goal fixation*, which in a living animal have an important influence on volition.

In implementing such simulations of nervous activity, it is of course impracticable to include a counterpart of every cell that is active in the animal cortex, but it is possible to include representatives of cells of the various types of excitatory and inhibitory cells, and the resulting computer simulations are in most respects remarkably realistic.

8.5 Theory of Consciousness

Shannon's development of a classical theory of information represented a significant contribution not only to the theory of probability but to the understanding of thermodynamics and statistical physics, especially through the interpretation of entropy as microscopic information to be gained. However, quite apart from the fact that classical information was conceived as

a purely numerical quantity without any indication of what the information was about, it also left untouched the mystery of how an actual event to which only a numerical probability could be attached becomes certain through its realization by a conscious observer. To unravel this mystery it would seem to be necessary to understand how the effect of an event on the brain of the observer is different from the lasting impression it makes elsewhere in the physical world.

The brain is composed of matter not essentially different from other physical systems, so to suppose that it was subject to different laws would be merely to compound the mystery. Throughout the era of classical physics, the problem was recognized but never satisfactorily resolved. However, following the discovery of quantum mechanics and its interpretation as an indeterministic theory, it occurred to many different people that if quantum physics could be implicated in some aspects of the functioning of the brain, then there could be some hope of understanding and explaining the nature of consciousness, and with it the apparently singular role played by the conscious observer in the processing of information. In the earlier sections of this chapter we have summarized the principal neurobiological facts and physical considerations that are relevant to the discussion to follow, and we shall now bring them together to summarize the physically based theory presented in detail in our book "Sources of Consciousness".

We must first give useful working definitions of consciousness and its correlates, noting that the importance of precise definitions is that, in their absence, much confusion can arise from the use of language by different people who entertain vague, ambiguous or mutually contradictory ideas about the meaning of certain words.

Definitions

- *Consciousness* is a synthesis of awareness and volition.
- *Awareness* is the acquisition of information.
- *Volition* is the creation of new information.

In science generally informal definitions are often to be preferred to those taken from a dictionary because they need not be circular or limited to a few words, and can be supplemented by mathematically formulated statements whose meaning is, or should be, independent of the speaker or reader. In the mathematical and physical sciences, precision often requires that technical meanings should be given to words taken originally from common speech, and in the more abstract branches of mathematics the meanings are sometimes only distantly related to those of ordinary usage. In the physical sciences, there is more insistence that technical meanings should be at least consistent with more generally accepted standards, and the above definitions are intended to conform with this requirement.

The formal definition that we have adopted of consciousness is in fact consistent with ordinary (non-scientific) usage. We note that, according to a widely used dictionary, consciousness is "awareness" or "the totality of conscious states, as of an individual", "*aware* usually implies vigilance in observing or in drawing inferences from what one sees, hears, etc.", and volition is the "act of willing or choosing" or "a state of decision or choice", while information is "knowledge derived from reading, observation or instruction; especially, unorganized facts or data". The dictionary definitions of consciousness, awareness and volition, though not identical with those given above, may be freely accepted as interpretations of their meaning. But, as is evident in earlier chapters of this book, the traditional meaning of the word 'information' has inevitably evolved to not only include electronically coded facts or data but facts or data derived from physical systems of any kind. Moreover, since the development of classical information theory, a quantitative measure has existed for macroscopic information, and with the development of quantal information theory it has become possible to identify information as a particular observable that, like other observables, can be expressed in terms of qubits. All of this is implicit in the above formal definitions adopted of awareness and volition.

With the help of a clear concept of the nature of consciousness, it becomes possible to identify the features of the nervous system of an animal that are required and are actually responsible for conscious behaviour. This is obviously an essentially preliminary step to the modelling, simulation, and eventually the reproduction of this behaviour, and the development of new devices for information processing that allow the essential features of consciousness to be realized independently of the nervous system.

We shall conclude by summarizing those aspects of the theory of consciousness presented here which are needed for these purposes. In Sect. 8.2 we have characterized the animal cortex as a quantal Turing machine, though obviously not one well adapted to perform reliable and reproducible computation. As a computing machine it could be described as well designed to compute the uncomputable, in the sense that the output is largely unpredictable. Nevertheless, like every Turing machine it is equipped with a 'tape', providing information to a 'machine' in the form of excitations of the extracellular fluid. The actual machine consists of neurons that are able to 'scan' and so gain designated information from the tape, and also to modify the 'tape' in such a way that its informational content is affected. Though the mode of operation of the machine need not be specified in detail, each operation on the tape is affected by its state as well as by the information derived from the tape. The state of the machine admits of a macroscopic description and is changed with each operation in an essentially deterministic way. This entails that the machine possesses some type of memory, and leads us to infer that memory is a significant, if not essential, asset to the functioning of the machine.

In its conscious activity the cortex must be characterized as a quantal, rather than a classical Turing machine because the tape consists of qubits rather than classical bits, and the scanning and modification of the tape are initiated by quantal rather than classical processes. But while the description of the cortex as a quantal computer is a valid one, it has several other characteristics and more detailed descriptions are not only possible but needed. To highlight its conscious functions, it is necessary to take note of the way in which quantal information is acquired and created by the cells of the cortex.

The conditions for quantal processes to have almost immediate macroscopic consequences have been emphasised in the first section of this chapter. In the animal brain they have been realized by the biological necessity to reduce the sodium and calcium concentrations of the cytoplasm of a cell far below that of the extracellular fluid, thus establishing an electrically and chemically metastable condition of the cellular membrane. The natural limits to the differences of the electrical and chemical potentials that can be sustained by the membrane have created conditions favourable for the transfer of information between neighbouring cells, and while much of this information processing is unconscious, it becomes conscious *if there are subsequent macroscopic developments that result in the formation of accessible sequential memory of information gained.* But the passive acquisition of information is not sufficient for the display of consciousness, and it is the capacity of the brain to create new information that is the most obvious manifestation of conscious behaviour, from the point of view of the external observer. It is an almost incidental feature of the transfer of information across the neural membrane that it is a two-way process and that the gain of information by a neuron is accompanied by the creation of information in the extracellular fluid which, assuming that it has observable and therefore macroscopic consequences, is according to our definition a requirement of consciousness.

The capacity of the brain to form accessible sequential memory of sensory information is a very important but variable requirement. Under some pathological conditions in which information is not processed by the hippocampus, memory fades after a few seconds and this is a severe handicap to the afflicted animal, which is nevertheless still recognized as conscious. The ability to form long-term memory requires not only the continual acquisition and generation of information, but the means of storing and retrieving it. The storage and retrieval of information depends on the sensitization and development of synapses resulting from long-term potentiation. It is largely an unconscious activity, but certainly an invaluable one from the point of view of natural selection, and it is not surprising that the hippocampus is part of the allocortex, the most primitive subdivision of the animal brain.

Information gained by awareness of sensory stimuli is objective in the sense that it corresponds to macrosopic physical processes in the brain. The acquisition of information is effected by physical processes, including long term potentiation and the consequent enhancement of specific synaptic con-

nections within the cortex. Following this largely unconscious activity, the cells affected are left in a state of significantly lower entropy than before. This change can be detected in principle by an external observer from the examination of EEG and MEG records, by its effect on behaviour, in retrieval from memory and conversation, or finally by invasive techniques such as autopsy.

The present theory of consciousness suggests various possibilities for the creation of artificial consciousness. Though the complexity of the animal brain would be hard to emulate, the actual physical processes that have been exploited by nature in the evolution of conscious beings are not intrinsically complex or impossible to reproduce. Also, some of these processes have various analogues that have already been proposed or are actually in use. Since the creation of information is not restricted to the animal cortex, it is worth examining the conditions under which awareness and volition could be expected to appear and be recognized outside the animal cortex. This will be done in the final section to conclude this chapter.

8.6 Consciousness in Nature

The concept of consciousness provides a broad avenue from physics to the most distant reaches of human thought and belief. The theory of consciousness presented in the last section was physically based but also had a strong bias towards quantal information theory; its application to the animal observer was transparent and inevitable in the light of our present experimental and theoretical knowledge of the external world. But traditionally the concept of consciousness has been linked with extensive areas of humanistic studies, including biology and psychology but also some which were so far removed from physics that they seemed to most early authorities to belong to an entirely different order of experience, notably philosophy and religion. In the twentieth century the earlier lines of demarcation between physics and philosophy have been eroded by the development of widespread interest in the philosophy of physics, and there have also been sporadic but important attempts to bridge the gulf between science and religion from both sides of the divide, for instance by de Chardin from the direction of religious thought and by Margenau from the direction of physics.

We have noticed that physics is not without its topics of controversy, especially those surrounding the interpretation of quantum mechanics, and in this volume have tried to show how the application of information theory, and especially of quantal information theory, can at least isolate those aspects of theoretical physics based firmly on our shared experience of the external world from elements that are subjective, though appealing strongly to the imagination and without doubt indispensable to the progress of science. There are clear benefits, however, to be derived from the recognition that the subjective

elements are a matter of personal preference and should not be allowed to become centres of disruptive or violent controversy. This was recognized by the most eminent of the theoretical physicists of the century, including those like Einstein and Schrödinger who chose in their different ways to dissent from the orthodox interpretation of quantum mechanics. To the author, who had the privilege of personal acquaintance with nearly all the great authorities of quantum theory, it seemed that the dissenters were distinguished from the orthodox Göttingen and Copenhagen schools by a mathematical preference for analytical rather than algebraic methods. Analysis has always been and remains a most valuable mathematical tool in theoretical physics, especially in its traditional applications to macroscopic physics. However, even at a very elementary level, the concern of analysis with the infinite and its correspondingly higher level of abstraction engenders an attitude which is very different from that derived from the applications of the theory of matrices or the more abstract branches of algebra. Thus the differences between distinguished theoretical physicists, especially in the area of quantum physics, appear to be strongly correlated with their mathematical preferences. The preference given to elementary algebraic methods and orthodox interpretations in the present book is an almost inevitable consequence of the fundamental importance attached to information theory and the coding of information in terms of a countable set of bits or qubits. One of the advantages of this approach, apart from its inherent simplicity, is that it is most readily adapted to the development of existing computational methods and quantum computational methods in the future.

Thus those manifestations of dissent and controversy which have arisen in theoretical physics were ultimately the consequence of personal preferences, and not over the shared information derived from experiment and observation. But information theory now provides a most valuable means of isolating the optional subjective elements from those where agreement should easily prevail. It may now be enquired whether, with the development of a theory of consciousness, it is possible to do something to resolve the much more serious controversies which have arisen in the areas of philosophy, in its broadest sense, and in secular belief. In philosophy, there seems to be some recognition that personal preferences are to be found in topics related to language and semantics, and much less so in those closely related to science, though the controversies of physics have received plenty of attention and so have all aspects of the nature of thought and the human mind.

We shall therefore consider more particularly what a physically based understanding of the nature of consciousness can do to illuminate the divide between areas of disagreement in secular belief which are optional or subjective and those which are, or could be, a shared perception. A comparison of the various secular beliefs is hardly necessary to observe that they are all based to a considerable extent on reliance on some form of verbal or written human authority, often derived from antiquity. However, a widespread be-

lief in this authority is conditional on its apparent consonance with personal experience of the external world. There are two rather common features of secular teaching which from the present point of view are of paramount importance: the belief in an act of creation, and the belief in the existence of a conscious and intelligent being apart from and more universal than is identified with the human or animal species. These features are now well within the ambit of science and offer a basis for agreement at least as compelling as the present different interpretations of science at present allow.

There are of course well known differences in belief in the act of creation as a matter of history, and reliable evidence of events in the past tends be corrupted with passage of time, so that these could be difficult to resolve. But there can be no doubt about the creativity of the presently observed processes of nature and of human beings and animals as part of nature, and their unpredictability is one of the most potent sources of belief in the supernatural. A physically based theory of consciousness in animals is now ready to say how and to what extent consciousness is implicit in the universe of nature.

We have identified consciousness as a synthesis of awareness and volition. Both are sub-microscopic and quantum mechanical in origin but have macroscopic consequences leading to the formation of short term or long term memory. In animals, awareness implies the formation of memory of information, and volition the active creation of new information. Both are potentially objective as well as subjective processes. We shall see that there is a sense in which the entire universe is conscious in such terms. Events at the quantal level are continually or constantly the sub-microscopic cause of macroscopic phenomena which leave a permanent or semi-permanent record in the external world. The most obvious examples are the events associated with the functioning of man-made devices, such as Geiger counters for the detection of the decay of radioactive nuclei and the various types of chambers used to detect particles in accelerators and the cosmic radiation. But there is also a wide variety of naturally occurring phenomena that cannot be predicted and must ultimately be attributed to events at a sub-microscopic level. The most obvious examples are turbulence and convection, which over a period of time invalidate detailed meteorological prediction, but all macroscopic phenomena are subject to laws with some degree of non-linearity so that unavoidably incomplete information at a given time leads to almost complete uncertainty over a characteristic time scale. The time scale is long for the motion of the planets, but short for most types of chaotic phenomena which are notoriously difficult to predict in detail. There are theories of non-linear and chaotic processes that are not necessarily based on quantum mechanics, but today it is acknowledged that the quantum theory is fundamental and that events at the sub-microscopic level must play a part in the initiation of most unpredictable macroscopic phenomena. We conclude that unpredictability in nature is a manifestation of events subject to the laws of quantum mechanics.

It is thus difficult to deny the extension of the concept of awareness that has been developed in this chapter to phenomena other than those which have been identified in the animal brain. Natural events at the quantal level have macroscopic consequences, the memory of which resides in our environment and the universe at large. Volition, in the sense of the creation of new information, is also a common feature of natural phenomena, though devoid of the self-interest and primitive emotion that is all too evident in the higher animals. In inanimate nature there is no cell membrane that serves to differentiate cleanly between input and output, or awareness and volition, and the two are therefore more intimately related. But both are active throughout time and space, and the perception that this is so is not only justifiable but a most likely, though often unrecognized, source of religious belief. Stripped as it is of personal preferences which can at best be regarded as optional, the extended theory of consciousness offers a basis for agreement in areas which have hitherto been controversial and severely disruptive. The theory can be interpreted as one of continuous creation, not in the materialist sense of the creation of matter but in the unambiguous sense of the creation of information which is accessible to any observer.

In humans and other animals, consciousness is often associated with intelligence, but however the latter is defined the two are almost unrelated. Intelligence has various attributes, which may include sensitivity: the capacity to respond appropriately to external stimuli; impressibility: the capacity to form memory of past experience; plasticity: the capacity to adapt and learn from experience; activity: the capacity to perform tasks reliably and without supervision; and foresight: the ability to anticipate future developments, in so far as that is possible. Though these attributes may be displayed from time to time in the volitional activity of the human brain, they are more commonly realized in the operation of a well constructed computer program which does not require conscious intervention. By a process akin to natural selection, the classical computer has gradually acquired a level of artificial intelligence far surpassing that of the human brain in many areas. This has been a necessary prelude to what has been characterized as the next step in the process of evolution: the development of quantal computer programs with the basic requirements of self-reproduction and artificial consciousness. Already a symbiotic relationship has developed, between human beings and a computer network extending throughout most of the world and able to transfer and process information with superhuman speed and efficiency. The introduction of nodes of artificial consciousness into this network, operating on qubits instead of the bits of the classical Turing machine, could lead to the development of an ecological system endowed both with the best qualities evolved by natural selection and with an immeasurably greater intelligence and wisdom than is at present evident in human affairs.

A. Appendix: Matrices

A.1 Definitions and Elementary Properties

In the present context, a matrix a is a set of numbers (a_{11}, a_{12}, ... , a_{21}, a_{22}, ...) that can can be written as an array:

$$a = \begin{pmatrix} a_{11}\ a_{12}\ ... \\ a_{21}\ a_{22}\ ... \\ ...\ \ ...\ \ ... \end{pmatrix}, \tag{A.1}$$

with the element a_{jk} in the j-th row and k-th column. Two matrices a and b are regarded as equal ($a = b$) if their elements are the same ($a_{jk} = b_{jk}$ for all values of j and k). We shall consider only *square* matrices, with the same number of rows and columns. The number of rows and columns is then the order or *degree* of the matrices and may be any positive integer, or countably infinite.

The *trace* of the matrix a, denoted by $\mathrm{tr}(a)$, is the sum of the diagonal elements of a:

$$\mathrm{tr}(a) = a_{11} + a_{22} + ... = \sum_j a_{jj}. \tag{A.2}$$

If the degree of a is infinite, the trace is of course well defined only when the summation converges.

In a *complex* matrix each element a_{jk} is a complex number of the type $a^o_{jk} + \mathrm{i}a'_{jk}$, where a^o_{jk} and a'_{jk} are real numbers and i is the imaginary unit satisfying $\mathrm{i}^2 = -1$; the complex conjugate of a_{jk} is $a^*_{jk} = a^o_{jk} - \mathrm{i}a'_{jk}$.

There are various *conjugates* of matrix of a matrix a, of which the most fundamental are the transpose, the complex conjugate and the hermitean conjugate. The *transpose* of a is denoted by a^{t}, and is obtained from a by interchanging rows and columns:

$$a^{\mathrm{t}} = \begin{pmatrix} a_{11}\ a_{21}\ ... \\ a_{12}\ a_{22}\ ... \\ ...\ \ ...\ \ ... \end{pmatrix}, \tag{A.3}$$

so that $a^{\mathrm{t}}_{jk} = a_{kj}$. The transpose $(a^{\mathrm{t}})^{\mathrm{t}}$ of a^{t} is obviously the same as a. If $a^{\mathrm{t}} = a$, the matrix a is *symmetric*; if $a^{\mathrm{t}} = -a$, it is *anti-symmetric*. The

complex conjugate of a is denoted by a^*, and is obtained from a by replacing each element a_{jk} with its complex conjugate a^*_{jk}. If $a^* = a$, the matrix a is *real*; if $a^* = -a$, it is *imaginary*. The *hermitean conjugate* of a is denoted by $a^\dagger$, and is obtained from a by replacing each element a_{jk} with a^*_{kj}; from this it can be seen that $a^\dagger = (a^\mathrm{t})^* = (a^*)^\mathrm{t}$. If $a^\dagger = a$, the matrix a is *hermitean*; if $a^\dagger = -a$, it is *anti-hermitean*.

The *sum* of two matrices a and b with the same degree is the matrix

$$a + b = \begin{pmatrix} a_{11} + b_{11} & a_{12} + b_{12} & \ldots \\ a_{21} + b_{21} & a_{22} + b_{22} & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix}, \tag{A.4}$$

with $a_{jk} + b_{jk}$ in the j-th row and k-th column.

The *product* of a number λ and the matrix a is the matrix

$$\lambda a = \begin{pmatrix} \lambda a_{11} & \lambda a_{12} & \ldots \\ \lambda a_{21} & \lambda a_{22} & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix}, \tag{A.5}$$

with λa_{jk} in the j-th row and the k-th column.

The product of two matrices a and b with the same degree is the matrix

$$ab = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} + \ldots & a_{11}b_{12} + a_{12}b_{22} + \ldots & \ldots \\ a_{21}b_{11} + a_{22}b_{21} + \ldots & a_{21}b_{12} + a_{22}b_{22} + \ldots & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix}, \tag{A.6}$$

with

$$(ab)_{jk} = \sum_l a_{jl} b_{lk} \tag{A.7}$$

in the j-th row and the k-th column. A *summation convention* is in common use which omits the summation on the right side of the above equation, thus: $a_{jl}b_{lk}$, *on the understanding that a repeated affix such as l is to be summed over all admissible values.* In this volume, the 'Einstein' convention has been used sparingly and only when mentioned in advance.

The transpose $(ab)^\mathrm{t}$ of ab is $b^\mathrm{t}a^\mathrm{t}$, its complex conjugate $(ab)^*$ is a^*b^*, and its hermitean conjugate $(ab)^\dagger$ is $b^\dagger a^\dagger$. If the degree of the matrices is infinite, the product is well defined only when the summation converges. It is clear from this formula that, though $\mathrm{tr}(ab) = \mathrm{tr}(ba)$ when these traces are finite, ba is different from ab in general. Moreover, if the degree of a and b is infinite, $\mathrm{tr}(ab - ba)$ is in general different from zero. If $ab = ba$, the matrices a and b are said to *commute*, but the multiplication of matrices is not commutative in general. However, matrix multiplication is associative: $a(bc) = (ab)c = abc$, and matrices satisfy all other algebraic relations that do not require commutativity. The complex conjugate of the product ab is $(ab)^* = a^*b^*$, its transpose is $(ab)^\mathrm{t} = b^\mathrm{t}a^\mathrm{t}$ and its hermitean conjugate is $(ab)^\dagger = b^\dagger a^\dagger$. If a and b are symmetric, ab is not symmetric in general, but

$ab + ba$ is symmetric. Similarly, if a and b are hermitean, ab is not hermitean in general, but $ab + ba$ is hermitean and so is $\mathrm{i}(ab - ba)$.

Any matrix e which satisfies $e^2 = e$ is said to be *idempotent* or *projective*. The *unit* matrix, written as 1 in a matrix formula or equation, is

$$1 = \begin{pmatrix} 1 & 0 & \ldots \\ 0 & 1 & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix}, \tag{A.8}$$

with $1_{jk} = \delta_{jk}$ (defined as 1 if $j = k$, but 0 if $j \neq k$) in the j-th row and the k-th column. If a is any matrix with the same dimension, it follows from (A.7) that $1a = a = a1$. The unit matrix is projective and its trace is the degree of the matrix. The zero matrix, written as 0 in a matrix formula or equation, is also projective and its trace is of course zero.

A conjugate $\bar{a}$ of a may be formed with the help of any hermitean *conjugation matrix* $\bar{c}$ satisfying $\bar{c}^2 = 1$. The conjugate of a with respect to $\bar{c}$ is defined by

$$\bar{a} = \bar{c}a^\dagger\bar{c}, \qquad (c^\dagger = \mathrm{c}, \qquad \bar{c}^2 = 1). \tag{A.9}$$

If $\bar{a} = a$, the matrix a is *pseudo-hermitean*; then $\bar{c}a = a^\dagger\bar{c}$, so that $\bar{c}a$ is hermitean. The conjugate of the product ab with respect to $\bar{c}$ is $\bar{c}(ab)^\dagger\bar{c}$, or $\bar{c}b^\dagger a^\dagger\bar{c}$. If a and b are pseudo-hermitean, then $ab + ba$ and $\mathrm{i}(ab - ba)$ are both pseudo-hermitean.

The *inverse* of a matrix a, here denoted by a^{-1} if it exists, satisfies $aa^{-1} = 1$. If a has no inverse, we shall use the same notation a^{-1} for its *pseudo-inverse*, which satisfies

$$aa^{-1} = a^{-1}a, \qquad aa^{-1}a = a. \tag{A.10}$$

If $a^\dagger = (a^*)^\mathrm{t}$ is the hermitean conjugate of a matrix a, it follows from (A.7) that

$$\mathrm{tr}(aa^\dagger) = \sum_j \sum_k \mathrm{tr}(a_{jk}a^\dagger_{kj}) = \sum_j \sum_k (a_{jk}a^*_{jk})^2 \geq 0. \tag{A.11}$$

Moreover, the value 0 is possible only if $a = 0$; for this reason, the matrix $aa^\dagger$ is said to be *positive definite*. If a is hermitean, then $a^2 = aa$ is positive definite.

A.1.1 Direct Products and Vector Subscripts

It is often convenient to extend the notation in which a_{jk} is used to denote the element of a matrix a in the j-th row and k-th column, and to regard the subscripts j and k as vectors with components $(j_1, j_2, \ldots j_n)$ and $(k_1, k_2, \ldots k_n)$ respectively. This is true especially in the formation of the direct product of two or more matrices.

For two matrices $a^{[1]}$ and $a^{[2]}$ of degree d_1 and d_2, with elements $a^{[1]}_{j_1k_1}$ $(j_1, k_1 = 1, ...d_1)$ and $a^{[2]}_{j_2k_2}$ $(j_2, k_2 = 1, ...d_2)$, the *direct product* can be defined as a matrix $a = a^{[1]} \otimes a^{[2]}$ of the (d_1d_2)-th degree with elements

$$a_{jk} = (a^{[1]} \otimes a^{[2]})_{jk} = a^{[1]}_{j_1k_1} a^{[2]}_{j_2k_2}. \tag{A.12}$$

The subscripts j and k could be defined by $j = 2(j_1 - 1) + j_2$ and $k = 2(k_1 - 1) + k_2$ which would then take values from 1 to $d = d_1d_2$, but there are some advantages in regarding them as *vectors* $j = (j_1, j_2)$ and $k = (k_1, k_2)$ which still take d different values when their components take values from 1 to d_1 and from 1 to d_2, respectively. The matrix a can be added to and multiplied by other matrices of the d-th degree, and multiplied by numbers in the usual way, so that it is possible to express the direct product as an ordinary matrix product, by writing

$$a = a^{(1)}a^{(2)} = a^{(2)}a^{(1)} = a^{[1]} \otimes a^{[2]}, \qquad a^{(1)} = a^{[1]} \otimes 1, \qquad a^{(2)} = 1 \otimes a^{[2]}, \tag{A.13}$$

where $a^{(1)}$ and $a^{(2)}$ are then matrices of the d-th degree with elements $a^{[1]}_{j_1k_1}\delta_{j_2k_2}$ and $\delta_{j_1k_1}a^{[2]}_{j_2k_2}$ respectively.

Direct products can be formed in a similar way with any number of factors. The direct product of n matrices $a^{[1]}$, $a^{[2]}$, ... $a^{[n]}$, of possibly different degrees d_1, d_2, ... d_n, is of the $d = d_1d_2...d_n$-th degree and given by

$$a = a^{[1]} \otimes a^{[2]} ... \otimes a^{[n]} = a^{(1)}a^{(2)}...a^{(n)}, \tag{A.14}$$

where the matrix elements of a are explicitly

$$a_{jk} = (a^{[1]} \otimes a^{[2]} ... \otimes a^{[n]})_{jk} = a^{[1]}_{j_1k_1} a^{[2]}_{j_2k_2} ... a^{[n]}_{j_3k_3}.$$

and the subscripts $j = (j_1, j_2, ...j_n)$ and $k = (k_1, k_2, ...k_n)$ are vectors with d components. The factors

$$a^{(1)} = a^{[1]} \otimes 1 ... \otimes 1, \qquad a^{(2)} = 1 \otimes a^{[2]} ... \otimes 1, \qquad ... \qquad a^{(n)} = 1 \otimes 1 ... \otimes a^{[n]}. \tag{A.15}$$

of a are all of the d-th degree.

A.1.2 The Imaginary Unit as a Matrix

The imaginary unit i can be represented as a matrix and there is then a *complex conjugation matrix* c^* such that the complex conjugate of any complex number $\lambda = \lambda^o + \mathrm{i}\lambda'$ is the product $\lambda^* = c^*\lambda c^*$. The representation of i and c^* is the same as that given for the real matrices τ_0 and τ_1 in (2.14):

$$\mathrm{i} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \qquad c^* = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \lambda = \begin{bmatrix} \lambda^o & \lambda' \\ -\lambda' & \lambda \end{bmatrix}. \tag{A.16}$$

In a process similar to direct multiplication, a complex matrix of the d-th degree may therefore be converted to a real matrix of degree $2d$, by the substitution of submatrices of *one* of the following types:

$$a_{jk}(1) = \begin{bmatrix} a^o_{jk} & a'_{jk} \\ -a'_{jk} & a^o_{jk} \end{bmatrix}, \qquad a_{jk}(2) = \begin{bmatrix} a^o_{jk} + a'_{jk} & 0 \\ 0 & a^o_{jk} - a'_{jk} \end{bmatrix},$$

$$a_{jk}(3) = \begin{bmatrix} a^o_{jk} & a'_{jk} \\ a'_{jk} & a^o_{jk} \end{bmatrix} \tag{A.17}$$

When converted by the substitution of $a_{jk}(1)$ for a_{jk}, a complex matrix which is hermitean becomes real and symmetric, while by the substitution of $a_{jk}(2)$ or $a_{jk}(3)$ a simple matrix which is symmetric becomes real and remains symmetric.

A.2 Determinants

The *determinant* of a matrix a is a number, which can be expressed in terms of a in several different ways. In this section we introduce the usual definition in terms of the *permutation* symbol $\epsilon_{j_1j_2...j_d}$. This has a finite number of subscripts j_1, j_2, ... j_d, each of which may take any integral value between 1 and d and may be defined by

$$\epsilon_{j_1j_2...j_d} = \prod_{s=1}^{d-1} \prod_{r=s+1}^{d} \frac{(j_r - j_s)}{(r - s)}. \tag{A.18}$$

For $d = 3$, this gives

$$\epsilon_{j_1j_2j_3} = \tfrac{1}{2}(j_2 - j_1)(j_3 - j_1)(j_3 - j_2). \tag{A.19}$$

It is obvious from the definition that $\epsilon_{j_1j_2...j_d}$ vanishes if any pair of the subscripts have the same value, and it reduces to 1 if $j_1 = 1$, $j_2 = 2$, ... and $j_d = d$. But it also changes sign if any pair of subscripts is interchanged, so that $\epsilon_{j_1j_2...j_d} = 1$ if $(j_1, j_2, ... j_d)$ is an even permutation of the first d integers, but $\epsilon_{j_1j_2...j_d} = -1$ if $(j_1, j_2, ... j_d)$ is an odd permutation of the first d integers. The determinant $\det(a)$ of the matrix a can now be written as a sum of d^d terms (at most $d!$ of which are different from zero), as follows:

$$\det(a) = \sum_{j_1=1}^{d} \sum_{j_2=1}^{d} ... \sum_{j_d=1}^{d} \epsilon_{j_1j_2...j_d} a_{j_11} a_{j_22} ... a_{j_dd}. \tag{A.20}$$

It is easy to see that the determinant vanishes if two of its columns are identical, thus if $a_{j_11} = a_{j_12}$ and $a_{j_21} = a_{j_22}$, we have

$$\sum_{j_1=1}^{d}\sum_{j_2=1}^{d}\epsilon_{j_1 j_2 \ldots j_d}a_{j_1 1}a_{j_2 2} = -\sum_{j_1=1}^{d}\sum_{j_2=1}^{d}\epsilon_{j_2 j_1 \ldots j_d}a_{j_1 2}a_{j_2 1}$$

$$\equiv -\sum_{j_2=1}^{d}\sum_{j_1=1}^{d}\epsilon_{j_1 j_2 \ldots j_d}a_{j_2 2}a_{j_1 1},$$

and an expression which is equal to its negative must vanish. From (A.20) we may also infer that

$$\sum_{j_1=1}^{d}\ldots\sum_{j_d=1}^{d}\epsilon_{j_1\ldots j_d}a_{j_1 k_1}\ldots a_{j_d k_d} = \epsilon_{k_1 k_2 \ldots k_d}\det(a). \tag{A.21}$$

For this formula reduces to (A.21) when $k_1 = 1$, $k_2 = 2$, ... and $k_d = d$, and both sides change sign when any two of the subscripts k_1, k_2, ... k_d are interchanged.

From the last result we can easily show that the value of a determinant is not affected by the interchange of its rows and columns. We first multiply (A.21) by $\epsilon_{k_1 k_2 \ldots k_d}$ and sum over all values of k_1, k_2, ... k_d, obtaining

$$\sum_{k_1=1}^{d}\ldots\sum_{k_d=1}^{d}\sum_{j_1=1}^{d}\ldots\sum_{j_d=1}^{d}\epsilon_{k_1\ldots k_d}\epsilon_{j_1\ldots j_d}a_{j_1 k_1}\ldots a_{j_d k_d} = d!\det(a). \tag{A.22}$$

Now, if we interchange its rows and columns, a is changed to its transpose a^{t}, but on the left side the resulting replacement of $a_{j_1 k_1}\ldots a_{j_d k_d}$ by $a_{k_1 j_1}\ldots a_{k_d j_d}$ can be reversed by a simple interchange of the summation variables $k_1\ldots k_d$ and $j_1\ldots j_d$. It follows that $\det(a^{\mathrm{t}}) = \det(a)$.

It is also easy to show from the definition that the determinant $\det(ab)$ of the product of the two matrices a and b is the product of their determinants. For if we multiply (A.22) by $b_{k_1 1}b_{k_2 2}\ldots b_{k_d d}$ and sum the result over all d values of each of k_1, k_2, ... k_d, we have

$$\sum_{j_1=1}^{d}\sum_{j_2=1}^{d}\ldots\sum_{j_d=1}^{d}\epsilon_{j_1 j_2\ldots j_d}(ab)_{j_1 1}(ab)_{j_2 2}\ldots(ab)_{j_d d} = \det(a)\det(b),$$

or

$$\det(ab) = \det(a)\det(b). \tag{A.23}$$

The inverse a^{-1} of a matrix a, if it exists, can be constructed from $\det(a)$ and the *cofactors* of the elements of a in $\det(a)$. The cofactor $e_{kj}(a)$ of a_{jk} in $\det(a)$ is obtained from the left side of (A.21) by omitting the factor $a_{j_k k}$ and the summation over j_k, and substituting l for j_k in the remaining expression; for instance,

$$e_{1l}(a) = \sum_{j_2=1}^{d}\ldots\sum_{j_d=1}^{d}\epsilon_{l j_2\ldots j_d}a_{j_2 2}\ldots a_{j_d d}.$$

Then $\sum_{k=1}^{d}a_{jk}e_{kl}(a) = \det(a)$ if $j = l$, but is zero if j has any other value, since it reduces to a determinant with two equal columns. Thus we obtain the important result

$$ae(a) = \det(a)1, \tag{A.24}$$

where $c(a)$ is the matrix with the cofactors $c_{jk}(a)$ as elements, and 1 is the unit matrix. From this equation and its transpose it follows that

$$a^{-1} = e(a)/\det(a), \tag{A.25}$$

provided that the determinant does not vanish.

A.3 Eigenvalues of Matrices

If a is a matrix and there is a number a_r and a *non-vanishing* matrix e_r such that

$$ae_r = a_r e_r = e_r a, \tag{A.26}$$

then a_r is called an eigenvalue of a and e_r an *eigenmatrix* of a corresponding to the eigenvalue a_r. A non-vanishing column of e_r is called an *eigenvector* of a. If, as in (1.28), the matrix is expressed in *spectral form*, i.e., in terms of a complete set of projections g_r, thus

$$a = \sum_j a_j g_j, \qquad g_j g_k = \delta_{jk}g_j, \qquad \mathrm{tr}(g_j) = 1,$$

then $ag_r = a_r g_r$, so that the a_r are eigenvalues and the g_r are eigenmatrices. In this and the next section we shall develop some techniques for the determination of the eigenvalues and eigenmatrices of a matrix a, so as to reduce it to spectral form.

We suppose in this section that the degree d of the matrix a is finite, and introduce the function

$$f(x) = \det(x - a), \tag{A.27}$$

in which x is a real variable, converted to a matrix by multiplication with the unit matrix. From the definition (A.21) of a determinant it is clear that $f(x)$ is a polynomial of the form

$$f(x) = x^d + f^{(1)}x^{d-1} + \ldots + f^{(d)}, \tag{A.28}$$

in which the coefficients f_r of the powers x^{d-r} of x are numerical constants. By standard algebraic or numerical methods, the roots x_r $(r = 1, 2, \ldots, d)$ of the *characteristic equation* $f(x) = 0$ can be determined, and when this has been done, $f(x)$ can be expressed in the form

$$f(x) = \prod_r (x - x_r). \tag{A.29}$$

We can easily show that the x_r are the eigenvalues of the matrix a. For, if we substitute $x - a$ for a in (A.24), we have with the help of (A.27)

$$(x - a)e(x - a) = f(x), \tag{A.30}$$

and if we then substitute the value x_r for x, the right side of this equation vanishes and we are left with $ae_r = x_r e_r$, where $e_r = e(x_r - a)$. By comparison with (A.26), we see that $x_r = a_r$ and that the corresponding eigenmatrix e_r is made up of cofactors of the matrix elements of $x_r - a$ in the determinant defined in (A.27). From (A.27) and (A.29) it follows that

$$(-1)^d f(0) = \det(a) = \prod_r a_r, \tag{A.31}$$

i.e., the determinant of any matrix is the product of its eigenvalues. In particular, if κ is a constant, the eigenvalues of $1 + \kappa a$ are $(1 + \kappa a_r)$, and

$$\det(1 + \kappa a) = \prod_r (1 + \kappa a_r).$$

But from the definition of the determinant in (A.21) it can be seen that when $\det(1 + \kappa a)$ is expressed in powers of κ, the coefficient of κ is $\mathrm{tr}(a)$, so we have also

$$\mathrm{tr}(a) = \sum_r a_r, \tag{A.32}$$

i.e., the trace of any matrix is the sum of its eigenvalues.

Let us now express the matrix $e(x - a)$ in (A.30) as a polynomial in the matrix variable x:

$$e(x - a) = x^{d-1} + x^{d-2}e^{(1)} + \ldots + e^{(d-1)}, \tag{A.33}$$

where the coefficients $e^{(r)}$ of the powers x^{d-r-1} of x are of course also matrices. By comparing coefficients of x^{d-r} on the two sides of (A.30) we obtain

$$e^{(1)} - a = f^{(1)}, \qquad e^{(2)} - ac^{(1)} = f^{(2)}, \qquad \ldots, \qquad -ae^{(d-1)} = f^{(d)}, \tag{A.34}$$

and hence, by elimination of the $e^{(r)}$,

$$f(a) = a^d + f^{(1)}a^{(d-1)} + \ldots f^{(d)} = 0.$$

With the help of (A.34) this powerful result, due to Cayley, can also be written

$$f(a) = \prod_r (a - a_r) = 0 \tag{A.35}$$

showing that *any matrix a satisfies the same characteristic equation* $f(x) = 0$ *as its eigenvalues.*

A.3.1 Reduction of a Finite Matrix to Spectral Form

We shall first suppose that the eigenvalues a_r of the matrix a are all different; we shall see later that this is not an essential limitation. But then it follows from (A.32) and (A.35) that the matrices defined by

$$g_r = \prod_{s \neq r} [(a - a_s)/(a_r - a_s)] \tag{A.36}$$

have the following properties:

(1) each g_r is an eigenmatrix of a corresponding to an eigenvalue a_r;
(2) the *projective* condition $g_r^2 = g_r$ is satisfied; and
(3) if $s \neq r$, then $g_r g_s = 0$.
(4) Also, the g_r satisfy the algebraic identity $\sum_r g_r = 1$.
(5) Finally, we can show that, if g_r is hermitean or pseudo-hermitean, as defined in (A.9), then $\mathrm{tr}(g_r) \rangle 0$. For it follows from the projective condition that the eigenvalues of the g_r can only be 0 or 1, and they cannot all be zero, since then the eigenvalues of $g_r^\dagger g_r$ would also vanish, $\mathrm{tr}(g_r^\dagger g_r)$ would vanish by virtue of (A.32) and g_r itself would vanish by virtue of (A.11). Thus the $\mathrm{tr}(g_r)$ must all be positive integers, but from $\sum_r g_r = 1$ we have $\sum_r \mathrm{tr}(g_r) = d$, so that none of these integers can be greater than 1. To summarize, all the relations

$$g_r g_s = g_r \delta_{rs}, \qquad \sum_r g_r = 1, \qquad \mathrm{tr}(g_r) = 1$$

$$a = a \sum_r g_r = \sum_r a_r g_r, \tag{A.37}$$

showing that *any* finite matrix with distinct eigenvalues can be expressed in the form (1.13) assumed for an observable.

In a similar way, provided a numerical function $b(x)$ with the values $b(a_r)$ exists, a corresponding matrix function $b(a)$ of a matrix a can be defined by

$$b(a) = \sum_r b(a_r) g_r; \tag{A.38}$$

It is possible that two or more of the values $b(a_r)$ are equal, and this suggests a way of extending the results leading to (A.36) to an hermitean matrix b with two or more eigenvalues b_r that are not distinct. We simply express b as a function $b(a)$ of a second matrix a with distinct eigenvalues, the function chosen in such a way that the values $b_r = b(a_r)$ of the numerical function $b(x)$ are the same. Then b can be expressed in terms of the projections g_r of a, thus $b = \sum_r b_r g_r$.

The formula (A.38), with $b(a) = \log a$, can be used to obtain a useful expression for the determinant of the matrix a. According to (A.31), if any eigenvalue of a is zero, $\det(a)$ is zero, so that this possibility need not be considered. Also, according to (A.31) and (A.32),

$$\det(a) = \exp(\sum_r \log a_r) = \exp[\mathrm{tr}(\log a)] \tag{A.39}$$

A.3.2 Representation of Observables by Matrices

In quantum mechanics an observable is represented by a matrix a, whose eigenvalues a_r are possible results of a measurement of the observable. These eigenvalues must be real, and to ensure this is so it is sufficient, though not necessary, to require that a should be hermitean. More generally, the eigenvalues of a are real if a is *pseudo-hermitean*, so that there is an hermitean conjugation matrix $\bar{c}$ such that $\bar{c}a$ is hermitean, i.e., $\bar{c}a = a^\dagger \bar{c}$. For, assuming this, it follows from (A.26) that $e_r^\dagger a^\dagger = a_r^* e_r^\dagger$, where $e_r^\dagger$ is the hermitean conjugate and a_r^* the complex conjugate, so that

$$a_r e_r^\dagger \bar{c} e_r = e_r^\dagger \bar{c}(a e_r) = (e_r^\dagger a^\dagger)\bar{c} e_r = a_r^* e_r^\dagger \bar{c} e_r.$$

Since $\bar{c}^2 = 1$, $e_r^\dagger \bar{c} e_r = (e_r^\dagger \bar{c})(\bar{c} e_r)$ is positive definite and could only vanish if e_r were zero. But as e_r may not vanish, $a_r^* = a_r$, and a_r must be real. When $\bar{c} = 1$, a is not just pseudo-hermitean but hermitean.

There are, however, independent reasons for requiring that an observable in a particular inertial frame should be hermitean. In Sect. 5.5 it was shown that the conditional probability p_{rs} that the measurement of the observable $a = \sum_r a_r g_r$ will yield the value a_r, when it is certain that the measurement of a selected observable $\tilde{a} = \sum_k \tilde{a}_k \tilde{g}_k$ will yield the value $\tilde{a}_s$, is $p_{rs} = \mathrm{tr}(g_r \tilde{g}_s)$. It is important, therefore to ensure that $0 \leq \mathrm{tr}(g_r \tilde{g}_s) \leq 1$, and this can be done if it is assumed that g_r and $\tilde{g}_s$ are hermitean, i.e., that $\bar{c} g_r = g_r^\dagger \bar{c}$ and $\bar{c}\tilde{g}_s = \tilde{g}_s^\dagger \bar{c}$. For then it follows from (A.22) that

$$\mathrm{tr}(g_r \tilde{g}_s) = \tfrac{1}{2}\,\mathrm{tr}(g_r^2 \tilde{g}_s^2) = \mathrm{tr}(\tilde{g}_s g_r g_r \tilde{g}_s) = \mathrm{tr}[(\tilde{g}_s g_r)(\tilde{g}_s g_r)^\dagger] \geq 0,$$

$$1 - \mathrm{tr}(g_r \tilde{g}_s) = \tfrac{1}{2}\,\mathrm{tr}(g_r - \tilde{g}_s)^2 = \tfrac{1}{2}\,\mathrm{tr}[(g_r - \tilde{g}_s)(g_r - \tilde{g}_s)^\dagger] \geq 0,$$

and the necessary inequalities $0 \leq p_{rs} \leq 1$ are satisfied if both observables are represented by hermitean matrices, but not in general otherwise.

Finally, we shall now establish the existence of intertwining matrices h_{rs} and h_{sr} which connect any two projections g_r and g_s of $a = \sum_r a_r g_r$, thus:

$$g_r h_{rs} = h_{rs} g_s, \qquad h_{sr} g_r = g_s h_{rs}, \qquad h_{rs} h_{sr} = g_r. \tag{A.40}$$

If the representation chosen for a is diagonal, the matrix elements of g_r and g_s are $(g_r)_{jk} = \delta_{jr}\delta_{rk}$ and $(g_s) = \delta_{js}\delta_{sk}$, and those of h_{rs} and h_{sr} are then

$$(h_{rs})_{jk} = \delta_{jr}\delta_{ks}, \qquad (h_{sr})_{jk} = \delta_{js}\delta_{kr} \tag{A.41}$$

But if the chosen representation is not diagonal, suppose that b is any observable which, like a, is hermitean or pseudo-hermitean, but not a function

of a, so that $b_{rs} = g_r b g_s \neq 0$. Then $g_r b_{rs} = b_{rs} g_s$ and $b_{sr} g_r = g_s b_{sr}$. Also, from (A.9) it follows that $b_{sr} = g_s b g_r$ is the hermitean or pseudo-hermitean conjugate of b_{rs} so that $b_{rs} b_{sr}$ is positive definite and cannot vanish. Moreover, the spectral expansion of the observable $b_{rs} b_{sr}$ must consist of the single term $\mathrm{tr}(b_{rs} b_{sr}) g_r$, so that if

$$h_{rs} = b_{rs}/[\mathrm{tr}(b_{rs} b_{sr})]^{\frac{1}{2}}, \qquad h_{sr} = b_{sr}/[\mathrm{tr}(b_{rs} b_{sr})]^{\frac{1}{2}}$$
$$(b_{rs} = g_r b g_s, \qquad b_{sr} = g_s b g_r), \tag{A.42}$$

then all the required relations of (A.40) are satisfied.

A.4 The Factorization Method

We next describe the *factorization method* for the determination of the eigenvalues of an infinite hermitean matrix a, expressed in the spectral form

$$a = a^{(1)} = a_1 g_1 + a_2 g_2 + a_3 g_3 + \ldots. \tag{A.43}$$

The eigenvalues a_r of a are supposed to be bounded below, and are determined in numerically ascending order. The method relies on the construction of the sequence of matrices

$$a^{(r)} = a_r g_1 + a_{r+1} g_2 + a_{r+2} g_3 + \ldots \qquad (r = 1, 2, 3\ldots)$$

such that $a^{(r)} - a_r$ is positive definite but with a vanishing lowest eigenvalue. We note, with the help of (A.40), that the matrices of this type can be factorized into *codiagonal* matrices $\bar{c}_r$ and c_r, thus: $a^{(r)} - a_r = \bar{c}_r c_r$, where

$$\bar{c}_r = (a_{r+1} - a_r)^{\frac{1}{2}} h_{r+1,r} + (a_{r+2} - a_r)^{\frac{1}{2}} h_{r+2,r+1} + (a_{r+3} - a_r)^{\frac{1}{2}} h_{r+3,r+2} + \ldots \tag{A.44}$$

and is the conjugate of c_r. Then the eigenvalues a_r, and the matrices $\bar{c}_r$, c_r and the $a^{(r+1)}$ are successively determined by the relations

$$a^{(r)} = \bar{c}_r c_r + a_r, \qquad a^{(r+1)} = c_r \bar{c}_r + a_r. \tag{A.45}$$

In the diagonal representation of a, the h_{rs} have the simple matrix elements given in (A.41). From (A.44) and (A.40) it is evident that, for $s \geq r$, $\bar{c}_r g_s = g_{s+1} \bar{c}_r$, i.e., that $\bar{c}_r$ changes an eigenmatrix g_s to g_{s+1}. Similarly, c_r changes g_{s+1} to g_s.

The factors $\bar{c}_r$ and c_r of $a^{(r)} - a_r$ in (A.45) are not unique, and may be replaced by other matrices $\bar{c}_r \bar{u}$ and $u c_r$, if $\bar{u}$ and u satisfy the unitary or pseudo-unitary condition $\bar{u} u = 1$, but this change does not affect the eigenvalue. The particular factors chosen above ensure that $a^{(r+1)}$ commutes with $a^{(r)}$, but that feature is not essential for the success of the factorization

method and any sequence of factorizations consistent with (A.45) will yield the same eigenvalues.

The method for determining the eigenvalues therefore proceeds in general as follows. There are normally two values of a_1 which allow the matrix $a - a_1$ to be factorized into conjugate matrices $\bar{c}_1$ and c_1, and it is necessary to choose the *greater* of these values if the positive definite matrix $\bar{c}_1 c_1$ is to have a zero eigenvalue. Then a_1 will be the least eigenvalue of a, multiplied by the unit matrix, and $a^{(2)}$ is defined by (A.42) with $r = 1$. Next a_2 is chosen to allow $a^{(2)} - a_2$ to be factorized into conjugate matrices $\bar{c}_2$ and c_2, in such a way that $\bar{c}_2 c_2$ has a zero eigenvalue; then a_2 is greater than a_1 but is the least eigenvalue of $a^{(2)}$ and the second least eigenvalue of a, and $a^{(3)}$ is defined by (A.42). This step by step procedure could then be continued indefinitely, but in practice it is usually possible to obtain a general expression for c_r by induction, so that a general expressions can also be written down for $a^{(r)}$ and the r-th eigenvalue a_r. The eigenvalues may approach a finite limiting value a_∞, and there is then normally a continuous spectrum of eigenvalues extending above a_∞, of the type to be considered in the next section. If, however, there is no finite limiting value, all the eigenvalues of a are in the countably infinite sequence $(a_1, a_2, ...)$.

We note that from (A.45) it follows that $a^{(s+1)}\mathrm{c}_s = \mathrm{c}_s a^{(s)}$, so that

$$\bar{c}_1 \bar{c}_2 ... \bar{c}_r c_r ... c_2 c_1 = (a - a_1)(a - a_2)...(a - a_r) \qquad \text{(A.46)}$$

reduces to the same function $f(a)$ of a shown for finite matrices in (A.35). But here the sequence of eigenvalues does not terminate, so that the right side of (A.46) does not vanish identically. However, if $s \leq r$, the right side vanishes when multiplied by the eigenmatrix g_s, and it follows from this result that $c_r ... c_2 c_1 g_s = 0$.

A matrix observable, such as the energy H of a system in non-relativistic quantum mechanics, has an infinite set of eigenvalues and must therefore be represented by an infinite matrix. The eigenvalues of the energy have a lower bound, though possibly no upper bound, and may therefore be determined by a series of factorizations such as are described above. Several examples are given in Sect. 5.2, but here we illustrate this with simplest example, for the quantized harmonic oscillator with energy, coordinate and momentum observables H, q and p related by

$$H = (p^2 + m^2\omega^2 q^2)/(2m), \qquad qp - pq = \mathrm{i}\hbar, \qquad \text{(A.47)}$$

where the numerical constant m is the mass and ω is the classical frequency of the oscillator.

In this instance, it is easy to see that if H_1 is the least eigenvalue of H, the factors of $H - H_1$ must be multiples of $(p + \mathrm{i}m\omega q)$ and $(p - \mathrm{i}m\omega q)$, and the greatest of the two possible values $\pm\frac{1}{2}\hbar\omega$ for H_1 in (A.47) is achieved by taking

$$\bar{c}_r = \bar{c} = (p + \mathrm{i}m\omega q)/(2m)^{\frac{1}{2}}, \qquad c_r = c = (p - \mathrm{i}m\omega q)/(2m)^{\frac{1}{2}}, \qquad \text{(A.48)}$$

at least for $r = 1$. But, again in this particular instance, these are also factors for $r = 1, 2, ...$, since if $H^{(1)} = H$,

$$H^{(r)} = \bar{c}_r c_r + H_r, \qquad H^{(r+1)} = c_r \bar{c}_r + H_r, \qquad H_r = (r - \tfrac{1}{2})\hbar\omega \qquad \text{(A.49)}$$

for general values of r.

The above expressions for $\bar{c}$ and c are identical with those obtained from (4.33), with $\lambda = (\frac{1}{2}m\hbar\omega)^{\frac{1}{2}}$ as the unit of momentum. They are somewhat simplified by taking m and $\hbar\omega$ as units of mass and energy, and this will be done implicitly in the following section.

A.5 Continuous Eigenvalues

If q is an observable with an eigenvalue x that can have any real value between $-\infty$ and $+\infty$, it has no diagonal representation, but in suitable units there is an infinite matrix representation

$$q = \begin{bmatrix} 0 & 1 & 0 & 0 & ... \\ 1 & 0 & \sqrt{2} & 0 & ... \\ 0 & \sqrt{2} & 0 & \sqrt{3} & ... \\ 0 & 0 & \sqrt{3} & 0 & ... \\ ... & ... & ... & ... & ... \end{bmatrix}, \qquad \text{(A.50)}$$

in which the element in the c-th column and the r-th row is $q_{cr} = \sqrt{(c+1)}\delta_{r,c+1} + \sqrt{(r+1)}\delta_{r+1,c}$. A complementary observable is p, where

$$p = \tfrac{1}{2}\,\mathrm{i}\hbar \begin{bmatrix} 0 & -1 & 0 & 0 & ... \\ 1 & 0 & -\sqrt{2} & 0 & ... \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & ... \\ 0 & 0 & \sqrt{3} & 0 & ... \\ ... & ... & ... & ... & ... \end{bmatrix}, \qquad \text{(A.51)}$$

which is obviously hermitean; the matrices p and q satisfy the required relation

$$qp - pq = \mathrm{i}\hbar. \qquad \text{(A.52)}$$

We shall show that an analogue of the countable set of minimal projections g_r is the uncountable set g_x defined by

$$g_x = \frac{\mathrm{e}^{-\frac{1}{2}x^2}}{(2\pi)^{\frac{1}{2}}} \begin{pmatrix} [h_0(x)]^2 & h_0(x)\,h_1(x) & h_0(x)\,h_2(x) & h_0(x)\,h_3(x) & ... \\ h_1(x)\,h_0(x) & [h_1(x)]^2 & h_1(x)\,h_2(x) & h_1(x)\,h_3(x) & ... \\ h_2(x)\,h_0(x) & h_2(x)\,h_1(x) & [h_2(x)]^2 & h_2(x)\,h_3(x) & ... \\ h_3(x)\,h_0(x) & h_3(x)\,h_1(x) & h_3(x)\,h_2(x) & [h_3(x)]^2 & ... \\ ... & ... & ... & ... & ... \end{pmatrix} \qquad \text{(A.53)}$$

where the $h_j(x)$ are the hermitean polynomials, defined by

$$\exp[-\tfrac{1}{2}(x-y)^2] = \exp(-\tfrac{1}{2}x^2)\sum_{n=0}^{\infty} h_n(x)y^n/(n!)^{\frac{1}{2}} \tag{A.54}$$

It is easily verified that

$$h_0(x) = 1, \qquad h_1(x) = x, \qquad h_2(x) = (x^2-1)/(2!)^{\frac{1}{2}},$$

$$h_3(x) = (x^3-3x)/(3!)^{\frac{1}{2}}, \qquad h_4(x) = (x^4-6x^2+3)/(4!)^{\frac{1}{2}}, \qquad \ldots \quad .$$

Since the leading term in the polynomial $h_n(x)$ is proportional to x^n, these polynomials are linearly independent. By differentiating the equation (A.54) with respect to x, we obtain

$$n^{\frac{1}{2}}h_{n-1}(x) = h_n'(x). \tag{A.55}$$

But if we differentiate with respect to y, we have

$$(n+1)^{\frac{1}{2}}h_{n+1}(x) = xh_n(x) - n^{\frac{1}{2}}h_{n-1}(x). \tag{A.56}$$

From this it follows that

$$qg_x = xg_x = g_xq, \tag{A.57}$$

and similarly $qg_y = yg_y$, so that if $x \neq y$, $xg_xg_y = g_xqg_y = yg_xg_y$, and $g_xg_y = 0$. But for continuous variables we have $g_x^2 = Cg_x$, where

$$C = \sum_{n=0}^{\infty} \mathrm{e}^{-\frac{1}{2}x^2}[h_n(x)]^2$$

is divergent. By differentiating this formula for C with respect to x and using (A.55) and (A.56), we can verify that C is a constant, but on substituting $x = 0$, one gets a divergent series. Thus we need a new interpretation of the products of projections in the continuous spectrum; this is in terms of *distributions*.

From (A.55) and (A.56) we have

$$(n+1)^{\frac{1}{2}}h_{n+1}(x) = -\frac{d}{dx}[\mathrm{e}^{-\frac{1}{2}x^2}h_n(x)]$$

from which it follows by integration by parts that if

$$I_{m,n} = \frac{1}{(2\pi)^{\frac{1}{2}}}\int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}x^2}h_m(x)h_n(x)dx,$$

then $I_{n+1,n+1} = I_{n,n}$, so that, by mathematical induction, $I_{n,n} = I_{0,0} = 1$, and, by similar reasoning, $I_{mn} = 0$ when $m \neq n$. Thus

$$\int_{-\infty}^{\infty} g_x dx = 1, \tag{A.58}$$

(in which 1, as usual in a matrix equation, denotes the unit matrix). Thus,

$$g_xg_y = \delta(x-y)g_x, \tag{A.59}$$

where $\delta(x)$ is Dirac's delta-function, a distribution satisfying $\delta(x) = 0$ when $x \neq 0$ but

$$\int_{-\infty}^{\infty} \delta(x)dx = 1.$$

We can write

$$q = \int_{-\infty}^{\infty} xg_x dx, \qquad p = \mathrm{i}\hbar\int_{-\infty}^{\infty} d_xg_x dx, \tag{A.60}$$

where the elements of d_xg_x are

$$(d_xg_x)_{cr} = (2\pi)^{-\frac{1}{2}}\mathrm{e}^{-\frac{1}{2}x^2}[h_{c-1}(x)h_{r-1}'(x) - h_{r-1}(x)\,h_{c-1}'(x)], \tag{A.61}$$

in anti-hermitean form.

We can also introduce matrices g_{xy} defined by

$$(g_{xy})_{cr} = (2\pi)^{-\frac{1}{2}}\mathrm{e}^{-\frac{1}{4}(x^2+y^2)}h_c(x)h_r(y), \tag{A.62}$$

so that $g_x = g_{xx}$ and

$$g_{xu}g_{vz} = \delta(u-v)g_{xy}. \tag{A.63}$$

A.6 Parafermion Representations of Lie Algebras

In this section we discuss the matrix representations of the algebras named after the nineteenth century Norwegian mathematician Sophus Lie. A Lie algebra is a set of elements $(e_1, e_2, \ldots e_n)$ for any pair (e_a and e_b) of which a sum $e_a + e_b$ and a 'product' or commutator $[e_a, e_b]$ is defined, as well as the multiple λe_a of e_a by a number λ. The sum and the multiple satisfy the usual rules of commutative algebra, but the commutator is anti-commutative and non-associative, judged by the rules

$$[e_a, e_b] = -[e_b, e_a], \qquad [e_a, [e_b, e_c] + [e_b, [e_c, e_a] + [e_c, [e_a, e_b] = 0.$$

However, the elements can always be represented by matrices and when this is done the commutator has the form

$$[e_a, e_b] = e_ae_b - e_be_a. \tag{A.64}$$

Since this commutator is required to be an element of the algebra,

$$[e_a, e_b] = \sum_c C^c_{ab} e_c, \tag{A.65}$$

where the C^c_{ab} are called the *structure constants* of the Lie algebra. They are required to satisfy the *Jacobian identities*

$$C^c_{ab} = -C^c_{ab}, \qquad \sum_d (C^d_{ab} C^e_{dc} + C^d_{bc} C^e_{da} + C^d_{ca} C^e_{db}) = 0,$$

of which the latter follows from

$$[[e_a, e_b], e_c] + [[e_b, e_c], e_a] + [[e_c, e_a], e_b] \equiv 0.$$

A complete classification of the Lie algebras was made by E. Cartan, who found that there were varieties A_N, B_N, C_N and D_N, for all positive integral values of N, corresponding to the well known groups of unitary, odd orthogonal, symplectic and even orthogonal transformations $SU(N+1)$, $SO(2N+1)$, $Sp(2N)$ and $SO(2N)$ respectively, but also to some 'exceptional' varieties E_6, E_7, E_8, F_4 and G_2. As a matter of mathematical interest, we mention that the E varieties are related to the symmetries of the regular polyhedra, and F_4 and G_2 to those of Cayley's non-associative octonions. Here we shall discuss the representations of the Lie algebras in terms of the *parafermion creation and annihilation matrices* whose relevance to physics was first suggested by the author.

Parafermions are particles satisfying a generalized quantum statistics in which up to p dynamically indistinguishable particles, but no more, may coexist; p is called the *order of the parastatistics*. Thus, fermions are the parafermions of order 1. As individual particles, parafermions of order greater than 1 have never been and are unlikely to be observed, but particles like quarks of which a given number combine to form observable particles may be parafermions. But in the present context, the important application of the parafermion creation and annihilation operators is to the construction of the fundamental observables of physics in terms of elementary qubits.

A set of N parafermion creation and annihilation operators of order p can be constructed from Np matrices $\bar{f}^{(u)}_j$ and $f^{(u)}_j$ ($r = 1, 2, ...N$, $u = 1, ...p$) obtained by the factorization $n^{(u)}_j = \bar{f}^{(u)}_j f^{(u)}_j$ of the commuting projective matrices $n^{(u)}_j$ representing the constituent qubits of a tape, as described in Sect. 4.3. For different values of j and k or u and v, $\bar{f}^{(u)}_j$ and $f^{(u)}_j$ commute with $\bar{f}^{(v)}_k$ and $f^{(v)}_k$, but individually these matrices satisfy

$$\bar{f}^{(u)}_j f^{(u)}_j + f^{(u)}_j \bar{f}^{(u)}_j = 1, \qquad f^{(u)2}_j = \bar{f}^{(u)2}_j = 0. \tag{A.66}$$

As in Sect. 4.3, for each value of u a set of fermion creation and annihilation matrices $\bar{e}^{(u)}_j$, $e^{(u)}_j$ may be defined with the help of the $\xi^{(u)}_k = 2n^{(u)}_k - 1$ $(k = 1, ...j-1)$, where $\bar{e}^{(u)}_1 = \bar{f}^{(u)}_1$ and $e^{(u)}_1 = f^{(u)}_1$ but

$$\bar{e}^{(u)}_j = \bar{f}^{(u)}_j (\prod_{k=1}^{j-1} \xi^{(u)}_k), \qquad e^{(u)}_j = f^{(u)}_j (\prod_{k=1}^{j-1} \xi^{(u)}_k) \qquad (j > 1). \tag{A.67}$$

These matrices are of the 2^{pN}-th degree and satisfy the anti-commutation relations

$$\{e^{(u)}_j, \bar{e}^{(u)}_k\} \equiv e^{(u)}_j \bar{e}^{(u)}_k + \bar{e}^{(u)}_k e^{(u)}_j = \delta_{jk}, \qquad \{e^{(u)}_j, e^{(u)}_k\} \equiv e^{(u)}_j e^{(u)}_k + e^{(u)}_k e^{(u)}_j = 0,$$

$$\{\bar{e}^{(u)}_j, \bar{e}^{(u)}_k\} \equiv \bar{e}^{(u)}_j \bar{e}^{(u)}_k + \bar{e}^{(u)}_k \bar{e}^{(u)}_j = 0, \tag{A.68}$$

but if $u \neq v$, then $e^{(u)}_j$ and $\bar{e}^{(u)}_j$ commute with $e^{(v)}_k$ and $\bar{e}^{(v)}_k$. Finally, the parafermion creation and annihilation matrices are defined by

$$e^j = \sum_{u=1}^{p} \bar{e}^{(u)}_j, \qquad e_j = \sum_{u=1}^{p} e^{(u)}_j. \tag{A.69}$$

The number m_j of parafermions of the j-th type is the observable given by

$$m_j = \tfrac{1}{2} ([e_j, e^j] + p) = \tfrac{1}{2} \sum_{u=1}^{p} ([\bar{e}^{(u)}_j, e^{(u)}_j] + 1), \tag{A.70}$$

and as $[\bar{e}^{(u)}_j, e^{(u)}_j]$ has the eigenvalues -1 and 1, m_j has integral eigenvalues extending from 0 to p, as required.

Matrix representations of all of the basic Lie algebras can be constructed in terms of the conjugate elements e^j and e_j and

$$e^j_k = \tfrac{1}{2} [e^j, e_k] = \tfrac{1}{2} \sum_{u=1}^{p} [\bar{e}^{(u)}_j, e^{(u)}_k], \qquad e^{jk} = \tfrac{1}{2} [e^j, e^k] = \tfrac{1}{2} \sum_{u=1}^{p} [\bar{e}^{(u)}_j, \bar{e}^{(u)}_k],$$

$$e_{jk} = \tfrac{1}{2} [e_j, e_k] + \tfrac{1}{2} p = \tfrac{1}{2} \sum_{u=1}^{p} ([e^{(u)}_j, e^{(u)}_k] + \tfrac{1}{2}). \tag{A.71}$$

From the anti-commutation relations (A.68) we obtain the non-vanishing commutators

$$[e_j, e^k_l] = \delta^k_j e_l, \qquad [e^{jk}, e_l] = \delta^k_l e^j - \delta^j_l e^k, \qquad [e_{mj}, e^k_l] = \delta^k_j e_{ml} - \delta^k_m e_{jl},$$

$$[e^{jk}, e_{lm}] = \delta^k_l e^j_m - \delta^j_l e^k_m - \delta^k_m e^j_l + \delta^j_m e^k_l, \tag{A.72}$$

and others obtained by conjugation, or equivalently by interchanging subscripts and superscripts.

In terms of the parafermion algebra, the linearly independent elements of Lie algebras associated with groups of transformations are:

A_{N-1} or $su(N)$: e^j_k.

B_N or $so(2N+1)$: e^j_k, e^{jk}, e_{jk}, e^j and e_k.

C_N or $sp(2N)$: $e^j_k + e^{j+N}_{k+N}$, $e^j_{k+N} + e^k_{j+N}$ and $e^{j+N}_k + e^{k+N}_j$.

D_N or $so(2N)$: e^j_k, e^{jk} and e_{jk}.

Of the exceptional algebras, E_6 requires a set of 27 parafermion creation and annihilation matrices ($N = 27$), which will be denoted by $e^{(j,k,l)}$ and $e_{(j,k,l)}$ $(1 \le j,k,l \le 3)$; E_7 requires a set of 45 ($N = 45$), denoted by $e^{(jk,l)}$ and $e_{(jk,l)}$ $(1 \le j \ne k \le 6,\ 1 \le l \le 3)$; E_8 requires a set of 84 ($N = 84$), denoted by $e^{(jkl)}$ and $e_{(jkl)}$ $(1 \le j \ne k \ne l \le 9)$; F_4 requires a set of 18 ($N = 18$), denoted by $e^{(jk,l)}$ and $e_{(jk,l)}$ $(1 \le j,k \le 3,\ 1 \le l \le 3)$; and G_2 requires a set of 3 ($N = 3$), denoted by e^j and e_j $(1 \le j \le 3)$. In this notation, and with the summation convention applied to repeated affixes, the elements of the exceptional algebras may be listed as follows.

- E_6: $e^{(j,b,c)}_{(k,b,c)}$, $e^{(a,j,c)}_{(a,k,c)}$, $e^{(a,b,j)}_{(a,b,k)}$, $e^{(j,k,l)} + \epsilon^{jax}\epsilon^{kby}\epsilon^{lcz}e_{(a,b,c)(x,y,z)}$ and conjugates.
- E_7: $e^{(jb,x)}_{(kb,x)}$, $e^{(ab,j)}_{(ab,k)}$, $e^{(jk,l)} + \frac{1}{3}\epsilon^{jkabcd}\epsilon^{lyz}e_{(ab,y)(cd,z)}$ and conjugates.
- E_8: $e^{(jbc)}_{(kbc)}$, $e^{(jkl)} + \frac{1}{40}\epsilon^{jklabcxyz}e_{(abc)(xyz)}$ and conjugates.
- F_4: $e^{(jb;x)}_{(kb;x)}$, $e^{(ab;j)}_{(ab;k)}$, $e^{(jk;l)} + \frac{1}{3}\epsilon^{jab}\epsilon^{kcd}\epsilon^{lyz}e_{(ac;y)(bd;z)}$ and conjugates.
- G_2: e^j_k, $e^j + \epsilon^{jkl}e_{kl}$ and conjugates.

A Lie algebra ($\mathcal{L}_\infty$) is said to be *included in* another ($\mathcal{L}_\epsilon$), and we write $\mathcal{L}_\infty \subset \mathcal{L}_\epsilon$ if the linearly independent elements of $\mathcal{L}_\infty$ are fewer in number but can be expressed in terms of those of $\mathcal{L}_\epsilon$; thus, $G_2 \subset so(7)$ and $so(2N) \subset so(2N+1)$. Also, a matrix representation ($\mathcal{M}_\infty$) of a Lie algebra is said to be included in another representation ($\mathcal{M}_\epsilon$) of the same algebra if the non-vanishing matrix elements e_{rs} of any element e in the representation $\mathcal{M}_\infty$ are fewer in number but can be expressed linearly in terms of those of the same element e in $\mathcal{M}_\epsilon$.

A.6.1 Invariants and Representations of $so(2N+1)$

Since the elements of the Lie algebra $so(2N+1)$ are precisely those of the parafermion algebra, its matrix representations include representations of all the other Lie algebras. The representations of the 2^{pN}-th degree obtained are in general *reducible*, in the sense that they include L irreducible matrix representations of degree $(d_1, d_2, ...d_L)$, respectively, such that $\sum_l d_l = 2^{pN}$. An *irreducible* representation does not include any representation of lesser degree.

An *invariant* of a Lie algebra in any representation is a matrix which commutes with all elements of the algebra. A complete set of invariants (l_1, l_2, ... l_N) of $so(2N+1)$ may be defined as follows. First, for an irreducible representation l_1 is the maximum eigenvalue of m_1, given by (A.70), multiplied by the unit matrix; l_2 is the maximum eigenvalue of m_2, again multiplied by

the unit matrix, when m_1 already has its maximum eigenvalue, and so on; l_N is the maximum eigenvalue of m_N, multiplied by the unit matrix, when m_1, m_2, ... and m_{N-1} already have their maximum eigenvalues. Again in an irreducible representation, the l_j are called the *highest weights* of the representation, and it follows from (A.69) and their definitions that they have integral eigenvalues such that $p \ge l_1 \ge l_2 ... \ge l_N \ge 0$. However, for a reducible representation, l_j is defined as a diagonal matrix with the eigenvalue already defined within any included irreducible representation.

Any invariant of $so(2N+1)$ can be expressed in terms of the l_j, and there are invariants which can be expressed directly in terms of the elements of the Lie algebra. The most useful of these is

$$I = \tfrac{1}{2}\sum_j (e^j e_j + e_j e^j) + \sum_{j,k}(e^j_k e^k_j + e^{jk}e_{kj} + e_{jk}e^{kj}). \tag{A.73}$$

With the help of (A.72) we find

$$[e_l, I] = \sum_{j,k}[(e_k e^k_l + e^j_l e_j) + (e^k e_{kl} - e^j e_{lj}) + (e_{jl}e^j - e_{lk}e^k)]$$

$$+ \sum_j [(-e^j_l e_j + e^j e_{lj}) + (e_{lj}e^j - e_j e^j_l)] \equiv 0.$$

From this relation and its conjugate it follows that I is an invariant, known as the *quadratic invariant* of the algebra. We shall now express express this invariant in terms of highest weights.

For this purpose, let us suppose that in an irreducible representation with highest weights (h_1, h_2, ... h_N) the m_j are reduced to spectral form, thus:

$$m_j = \sum_r m_{jr} g_r \qquad (j = 1, 2, ...N). \tag{A.74}$$

According to (A.70), each of the m_j has integral eigenvalues m_{jr}, which in the irreducible representation considered extend from 0 to a maximum not exceeding l_1. There is a projection g_r corresponding to all admissible eigenvalues m_{jr} of the m_j, and if g_h is the projection corresponding to the highest weights, on multiplying (A.74) by g_h we have

$$m_j g_h = h_j g_h.$$

We note that, according to (A.70) and (A.71), the parafermion numbers are given by $m_j = e^j_j$, and from the commutation rules (A.72) it follows that if $j > k$ then

$$m_j e^j g_h = e^j(m_j + 1)g_h = (h_j + 1)e^j g_h,$$

$$m_j e^j_k g_h = e^j_k(m_j + 1)g_h = (h_j + 1)e^j_k g_h,$$

$$m_j e^{jk} g_h = e^{jk}(m_j + 1)g_h = (h_j + 1)e^{jk} g_h,$$

whereas if $N \geq l > j$ then

$$m_l e^j g_h = h_l e^j g_h, \qquad m_l e^j_k g_h = h_l e^j_k g_h, \qquad m_l e^{jk} g_h = h_l e^{jk} g_h.$$

But there is no eigenvalue $(h_j + 1)$ of m_j in this representation when the m_l with $l > j$ have the eigenvalues h_l, so that $e^j g_h$, $e^j_k g_h$ and $e^{jk} g_h$ must all be zero. Thus if $j > k$ then

$$e_j e^j g_h = 0, \qquad e^j e_j g_h = 2h_j g_h, \qquad e^k_j e^j_k g_h = 0, \qquad e^j_k e^k_j g_h = (h_j - h_k) g_h,$$

$$e^j_j e^j_j g_h = h^2_j g_h, \qquad e_{kj} e^{jk} g_h = 0, \qquad e^{jk} e_{kj} g_h = (h_j - h_k) g_h.$$

On substituting from (A.73), we can evaluate the eigenvalue of I on the eigenmatrix g_h, which is also the eigenvalue within the entire irreducible representation, thus:

$$I = h_N(h_N + 1) + h_{N-1}(h_{N-1} + 3) + ... + h_1(h_1 + 2N - 1). \qquad \text{(A.75)}$$

In the applications to quarks ($p = 3$) and particles with spin $\frac{1}{2}p$, the representation with highest weights $(p, p, ...p)$ is normally chosen, and I has the eigenvalue $Np(p + N)$.

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